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DIF3D: A CODE TO SOLVE ONE-, TWO-, AND THREE-DIMENSIONAL FINITE-DIFFERENCE DIFFUSION THEORY PROBLEMS

by

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PROGRAM ABSTRACT

1. Name of Program: DIF3D 4.0

2. Computer for which Program is Designed and Other Machine Version Packages Available: IBM 370 series, CDC 7600 and CRAY-1 computers.

3. Description of Problem Solved: DIF3D solves multigroup diffusion theory eigenvalue, adjoint, fixed source and criticality (concentration search) problems in 1-, 2- and 3-space dimensions for orthogonal (rectangular or cylindrical), triangular and hexagonal geometries. Anisotropic diffusion coefficients are permitted. Flux and power density maps by mesh cell and regionwise balance integrals are provided. Although primarily designed for fast reactor problems, upscattering and internal black boundary conditions are also treated.

4. Method of Solution: Mesh-centered finite-difference equations are solved by optimized iteration methods[1,2]. A variant of the Chebyshev semi-iterative acceleration technique is applied to outer (fission-source) iterations and an optimized block-successive-overrelaxation method is applied to the within-group iterations. Optimum overrelaxation factors are precomputed for each energy group prior to the initiation of the outer iterations. The forward sweep of the LU decomposition algorithm for the resulting tridiagonal matrices is computed prior to outer iteration initiation in orthogonal non-periodic geometry cases.

   In two- and three-dimensional hexagonal geometries the neutron diffusion equation is solved using a nodal scheme[3-5] with one mesh cell (node) per hexagonal assembly. The nodal equations are derived using higher order polynomial approximations to the spatial dependence of the flux within the hexagonal node. The final equations, which are cast in response matrix form, involve spatial moments of the node-interior flux distribution plus surface-averaged partial currents across the faces of the node. These equations are solved using a fission source iteration with coarse-mesh rebalance acceleration.

5. Restriction on the Complexity of the Problem: Problem dimensions are all variable. The number of mesh cells in a mesh plane is limited only by the available dynamic storage (see "Machine Requirements" below). In three-dimensional finite-difference problems a concurrent inner iteration strategy permits the specification of an unlimited number of mesh planes. Scattering is P_0 only and only CHI vectors are permitted.

The nodal option does not permit fixed-source problems. Enough core must be available on IBM machines to contain all data for at least one energy group. On the CDC 7600 machine, problem size may be limited by the requirement that one-group data for a single axial mesh plane fit in the available fast core memory.

6. Typical Running Time: Running time for the finite-difference calculation is roughly proportional to: flux work units (FWU) = number of space mesh cells x number of energy groups x number of iterations per group. Depending on the options selected, rates of 4 to 8 million FWU per minute on the IBM 370/195 are typical in three-dimensional problems. CPU times on the IBM 3033 are 35 to 50% greater than those obtained on the IBM 370/195. CPU times on the CDC 7600 are 10 to 25% less than those obtained on the IBM 370/195. CPU times on the CRAY-1 with the non-vectorized SLOR algorithm are about one-third those on the IBM 370/195. The vectorized SLOR algorithm times are nearly one-fourth those on the IBM 370/195.

   A three-dimensional nodal calculation with 4 energy groups and 14 axial mesh planes for a fast reactor model with sixth core planar symmetry and 17 rings of hexagons required approximately 1 CPU minute on an IBM 370/195 machine. The 6 triangle/hex finite-difference calculation for this same 14-plane problem required almost 2 cpu minutes. For accuracy comparable to the nodal option, the finite-difference calculation requires 42 mesh planes and 10 cpu minutes.

7. Unusual Features: The DIF3D nodal option uses a single meshpoint per hexagon instead of the six triangular meshpoints per hexagon typically employed in fast reactor finite difference calculations. The higher-order axial approximation[4,5] permits the use of coarse axial meshes without sacrificing accuracy. The nodal coupling coefficients are precomputed and stored only for unique nodes.

   DIF3D strictly adheres to the CCCC (Ref. 6) code standards and reads and writes CCCC interface datasets. For the finite-difference option more accurate peak power and peak flux edits are obtained by optionally calculating average power and flux values on mesh cell surfaces. The surface fluxes are obtained in a manner consistent with the mesh-centered finite-difference approximation.

8. Related or Auxiliary Programs: This is a stand-alone version of the DIF3D module described in Ref. 1-5. DIF3D is included in the REBUS-3 (Ref. 7) code package, and can thus be used to provide the neutronics solutions required in the REBUS-3 depletion calculations.

9. Status: The modular version of the code is in production use at Argonne. The standalone CDC 7600 and CRAY-1 versions of DIF3D are in production use at other laboratories.

10. References:

1. D. R. Ferguson and K. L. Derstine, "Optimized Iteration Strategies and Data Management Considerations for Fast Reactor Finite Difference Diffusion Theory Codes," Nucl. Sci. Eng., 64, 593 (1977).

2. K. L. Derstine,"DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite Difference Diffusion Theory Problems," ANL-82-64,Argonne National Laboratory, 1984.

3. R. D. Lawrence, "A Nodal Interface Current Method for Multigroup Diffusion Calculations in Hexagonal Geometry," Trans. Am. Nucl. Soc., 39, 461 (1981).

4. R. D. Lawrence, "A Nodal Method for Three-Dimensional Fast Reactor Calculations in Hexagonal Geometry," Proceedings of the Topical Meeting on Advances in Reactor Computations, Vol. II, p. 1030, Salt Lake City, American Nuclear Society, March, 1983.

5. R. D. Lawrence, "The DIF3D Nodal Neutronics Option for Two- and Three-Dimensional Diffusion Theory Calculations in Hexagonal Geometry," ANL-83-1, Argonne National Laboratory, 1983.

6. R. Douglas O'Dell, "Standard Interface Files and Procedures for Reactor Physics Codes, Version IV," UC-32 Los Alamos Scientific Laboratory (September 1977).

7. B. J. Toppel, "The Fuel Cycle Analysis Capability, REBUS-3," ANL-83-2, Argonne National Laboratory, 1983.

11. Machine Requirements: At least 325K-bytes of core storage are recommended for program and file buffer storage on the IBM 370 series. Between 30000 and 40000 words of SCM are required on the CDC 7600 depending upon the operating system employed. Additional (LCM on CDC) memory requirements expand linearly with the number of cells (N) in a mesh plane. The finite-difference option requires at least 9N (8-byte) words in 2-D problems and at least 25N words are required in 3-D problems. At least 19 mesh lines of data and one group of cross section data must be stored in SCM on the CDC 7600. External data storage must be available for approximately 40 scratch and interface files. Fourteen of these are random access scratch files (grouped into 6 file groups), the remainder are sequential access files with formatted or unformatted record types.

12. Programming Languages Used: The standard FORTRAN described in ANS STD.3-1971 is used. The program can be executed entirely in FORTRAN, except for dynamic memory allocation routines on IBM and CDC computers, random access I/O routines on IBM computers, and LCM/SCM transfer routines on the CDC 7600. The exceptions noted above are either written in assembly language or supplied from the CDC or CRAY system libraries. Thus non-Fortran code is about 2% of the IBM package and about .2% of the CDC and CRAY package.

13. Operating System: No special requirements are made of the operating system. The IBM linkage editor and the CDC or CRAY-1 overlay or segmented loading facilities may be used. Random access I/O data files should be supported for efficient operation, but they are not necessary for correct operation.

14. Other Programming or Operating Information or Restrictions: An optimized assembler version of the (finite-difference) tridiagonal matrix solution and overrelaxation routine is available for the CDC and CRAY systems. DIF3D is maintained as a single unified source file. Particular machine versions are configured at distribution time via activation and deactivation of coding bracketted by in-stream language flag comment cards.

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Major contributions to the finite-difference option of DIF3D were made by D. R. Ferguson.

16. Material Available: Restricted Distribution Magnetic Tape Transmittal

a) User's Manual

b) Magnetic Tape Containing

i) Source Code

ii) Sample Problem Data Card-Images

iii) Sample Problem Output

iv) Code Dependent BCD and Binary Card-Image File Descriptions

v) Linkage Editor, Segmented Loader or Overlay Loader Control Card-Images

vi) JCL Procedure for Execution.

17. Category: C

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ABSTRACT

The mathematical development and numerical solution of the finite-difference equations are summarized. The report provides a guide for user application and details the programming structure of DIF3D. Guidelines are included for implementing the DIF3D export package on several large scale computers.

Optimized iteration methods for the solution of large-scale fast-reactor finite-difference diffusion theory calculations are presented, along with their theoretical basis. The computational and data management considerations that went into their formulation are discussed. The methods utilized include a variant of the Chebyshev acceleration technique applied to the outer fission source iterations and an optimized block successive overrelaxation method for the within-group iterations.

A nodal solution option intended for analysis of LMFBR designs in two- and three-dimensional hexagonal geometries is incorporated in the DIF3D package and is documented in a companion report, ANL-83-1.

1. INTRODUCTION

This report is a user's manual for DIF3D, a computer code which uses the mesh-centered finite-difference approximation to obtain numerical solutions of the multigroup diffusion equations in one-, two- or three-dimensions for fast reactor applications. Although two mesh-centered finite-difference codes 3DB (Ref. 8) and VENTURE (Ref. 9) were already in existence, DIF3D (Ref. 1) was written to employ the more rigorous strategies of the well-known PDQ-7 (Ref. 10) code. This decision was based on a thorough intercomparison of several iterative strategies, the results[11] of which indicated the iterative method employed by PDQ-7 (Refs. 12 and 13), when modified to take advantage of several unique aspects of fast reactor diffusion theory calculations, is also highly efficient when applied to fast reactor calculations. Significant efforts were concurrently expended to provide efficient, yet flexible, data management and data structures in DIF3D. The numerical results in Ref. 1 demonstrate the efficiency achieved by these methods.

User interaction with the DIF3D acceleration and data management strategies principally involves only two parameters; ϵ_{in}, the inner iteration error reduction factor, and ECMSIZ, the ECM container size. For most problems the ϵ_{in} default is suitable and ECMSIZ is readily estimated. Optimizing the job cost for a class of similar problems involves only a simple adjustment to ϵ_{in} and ECMSIZ.

Incorporated in DIF3D for the solution of two- and three-dimensional hexagonal geometry problems is a nodal option that uses input data virtually identical to that of the finite-difference option. Reference 5 discusses the mathematical development and numerical solution of the nodal equations; some numerical comparisons between the nodal and finite-difference options for typical heterogeneous core LMFBR designs have shown that the accuracy of the nodal solution is superior to that of a standard (6 mesh cells per hexagon, 5 cm axial mesh) finite difference calculation, and that this improved accuracy is achieved with a potential order-of-magnitude reduction in computational cost for a three-dimensional calculation.

DIF3D was developed at Argonne National Laboratory and is operational on both the IBM 370/195 and the IBM 3033 computers, and is a principal module in the ARC System providing eigenvalue and flux calculations for the burnup code REBUS-3 (Ref. 7), the perturbation theory code VARI3D[14] and the flux synthesis code SYN3D[15] in addition to performing standalone neutronics calculations including nuclide concentration searches. The programming adheres strictly to the conventions set forth by the Committee on Computer Code Coordination[6] (CCCC). Most of the data for a calculation must be supplied in the format of the Standard Interface Files[6] defined by the CCCC. BCD input data (when it is required) is limited to data that is essential for the problem (i.e. redundant information is not required), and this data may be readily specified in free format. Particular attention has been paid to maintaining a single unified source in which language flag comment cards segregate code by particular and generic machine environments. A simple preprocessor code activates or deactivates language flags appropriate to the target machine environment. The portability afforded by this approach is demonstrated by the relative ease to which DIF3D is now exported and currently operational in standalone form on IBM 370 series computers, on CDC 7600 computers and on CRAY-1 computers.

The computational efficiency and data management flexibility (achieved with minimal user control), the user-oriented input data philosophy and the highly portable export package combine to make DIF3D an efficient computational tool that is a standard for the LMFBR community. Thermal reactor applications are routinely solved with DIF3D, also.

An overview of the major code block (modules) in the DIF3D package is provided in Fig. 1.1. DIF3D features are summarized in the code abstract on page xii. This report is organized into 5 sections. Section 2 provides users with the mathematical and computational aspects that strongly influenced the implementation of the optimized iteration strategies in DIF3D. Sections 3 and 4 respectively provide user and programmer information. Section 5 is intended for users who have just received DIF3D from the National Energy Software Center (NESC) and who are faced with the task of making the code operational on their machine; it describes the contents of the NESC tapes and outlines the steps necessary to implement DIF3D in stand-alone form on the IBM 370 series, the CDC 7600 and the CRAY-1 computers.

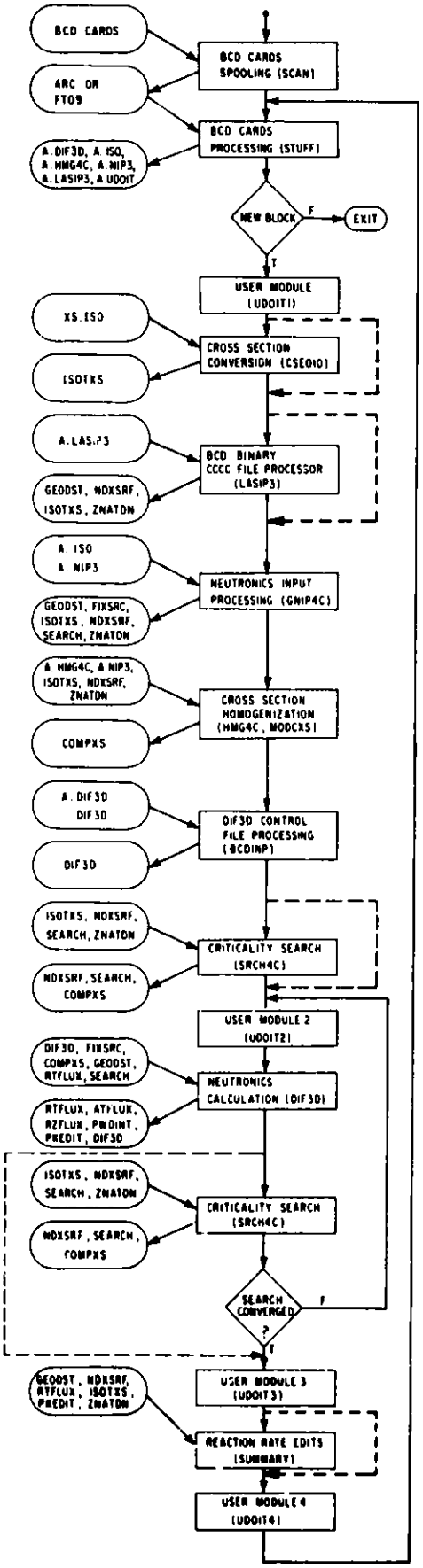

Fig. 1.1. Major Modules in the DIF3D Standard Path STP021

2. NEUTRONICS EQUATIONS AND SOLUTION METHODS

In this section, the "mesh-centered" finite-differenced form[16,17] of the multigroup neutron diffusion equations is presented and is accompanied by a review of the properties of these equations that permit the application of the iterative methods chosen to solve these equations. Theoretical aspects of the iterative methods are described and the computational and data management considerations that strongly influence the implementation of the iterative methods are discussed in turn. The equations which form the basis of the criticality search are also discussed.

2.1 Derivation of the Mesh-Centered Finite-Difference Equations

The mesh-centered form of the finite-difference equations rather than the mesh-edged form[10,13,18] is traditionally used in fast-reactor analysis because of the computational savings afforded in the calculation of the removal and source terms in Eqs. (2.1) and (2.2).

2.1.1 The Multidimensional Multigroup Neutron Diffusion Equations

In the mesh-centered finite-difference approximation the problem domain R is subdivided into a regular array of mesh cells such that all material interfaces lie on mesh cell surfaces. Within any mesh cell, say R_ℓ, the material properties are assumed homogeneous and the time-independent multigroup neutron diffusion equation[19] for mesh cell R_ℓ can then be written:

$$-\nabla\cdot D_\ell^g \nabla\phi_\ell^g(\underline{r}) + \Sigma_\ell^{r,g}\phi_\ell^g(\underline{r}) = Q_\ell^g(\underline{r}),\ \underline{r}\in R_\ell,\ g = 1,2,\ldots,G \tag{2.1}$$

where

$$Q_\ell^g(\underline{r}) \equiv \frac{1}{\lambda}\chi_\ell^g \sum_{g'=1}^{G} \nu\Sigma_\ell^{f,g'}\phi_\ell^{g'}(\underline{r}) + \sum_{g'\neq g} \Sigma_\ell^{s,gg'}\phi_\ell^{g}(\underline{r}) + S_\ell^g(\underline{r}), \tag{2.2}$$

λ denotes an eigenvalue, $S_\ell^g(\underline{r})$ denotes an optional distributed source, and the remainder of the notation is standard.[19,*]

Equation (2.1) is solved subject to the conditions that the flux and surface-normal component of the net current be continuous across cell interfaces, i.e.

$$\phi_\ell^g(\underline{r}) = \phi_m^g(\underline{r}) \tag{2.3}$$

$$\hat{n}\cdot D_\ell^g \nabla\phi_\ell^g(r) = \hat{n}\cdot D_m^g \nabla\phi_m(\underline{r}) \tag{2.4}$$

---

*Homogenization formulas defining the macroscopic cross section quantities appearing in Eq. (2.1) and Eq. (2.2) are defined in Section 3.6. Note that DIF3D permits χ-vectors, only; χ-matrices are not permitted.

for $\underline{r}$ on the interface between cells R_ℓ and R_m. Similar relations hold for the interfaces between R_ℓ and its remaining adjoining mesh cells.

Boundary conditions of the general form

$$\alpha^g \hat{n}\cdot D_\ell^g \underline{\nabla}\phi_\ell^g(\underline{r}) + \beta^g \phi_\ell^g(\underline{r}) = 0, \qquad \underline{r} \in \partial R, \tag{2.5}$$

are specified on cell surfaces which form part of the external boundary ∂R of R. Standard boundary conditions (e.g. zero flux, zero incoming partial current and extrapolated) are obtained via appropriate specification of the surface-dependent boundary constants α^g and β^g in Eq. (2.5).

When $S_\ell^g(\underline{r}) \equiv 0$ for all ℓ and g, Eq. (2.1), Eq. (2.2) and Eq. (2.5) define the eigenvalue problem for which the fundamental eigenvalue (k-effective) and eigenvector (neutron flux) are sought. Fixed source problems arise when $S_\ell^g \neq 0$ and λ is fixed at a user specified value ensuring reactor subcriticality. The corresponding flux solution is then sought.

Adjoint eigenvalue and fixed source problems determine the solution to the adjoint system associated with Eq. (2.1), Eq. (2.2) and Eq. (2.5).

2.1.2 The Orthogonal XYZ Geometry Derivation

The mesh-centered finite-difference equations will be derived in XYZ geometry for R_ℓ, an arbitrary mesh cell chosen from the IxJxK parallelepiped mesh cells defined by the coordinates $x_i, i=1,2,\ldots,I+1$, $y_j, j=1,2,\ldots,J+1$ and $z_k, k=1,2,\ldots,K+1$. The dimensions of R_ℓ are denoted by

$$\Delta s_\ell = s_{\ell+1} - s_\ell \quad \text{for} \quad s_\ell \equiv (x_i, y_j \text{ or } z_k). \tag{2.6}$$

Using a local coordinate system with the origin at the centroid of the mesh cell, R_ℓ is defined by

$$R_\ell \equiv R_{ijk} = \{\underline{r} = (x,y,z) \,\big|\, s = (x,y \text{ or } z) \in [-\Delta s_\ell/2,\ \Delta s_\ell/2]\}$$

The group index will be henceforth omitted and whenever possible the single subscript notation ℓ and m will denote R_{ijk} and adjacent cell, say, $R_m \equiv R_{i+1jk}$, respectively.

We start by integrating the neutron diffusion equation over the volume of R_ℓ, i.e. we operate on Eq. (2.1) with

$$\int_{r\in R_\ell} d^3r \cdot \equiv \int_{-\Delta z_k/2}^{\Delta z_k/2} dz \int_{-\Delta y_j/2}^{\Delta y_j/2} dy \int_{-\Delta x_i/2}^{\Delta x_i/2} dx \cdot . \tag{2.7}$$

Application of Gauss' Theorem to the integrated leakage term yields

$$\int_{\underline{r}\in R_\ell} d^3r\ \underline{\nabla}\cdot D_\ell \underline{\nabla}\phi_\ell(\underline{r}) \;=\; \sum_{p=1}^{6} \bar{J}_\ell^p A_\ell^p \tag{2.8}$$

where A_ℓ^p denotes the surface areas of R_ℓ with outwardly directed surface normal $\hat{n}_p$ (i.e. $\hat{n}_1 = -\hat{u}_x$, $\hat{n}_2 = \hat{u}_x, \ldots, \hat{n}_6 = \hat{u}_z$) and $\hat{u}_s$ denotes a unit vector in direction s. The resulting neutron balance equation may be written for each energy group in the form

$$\sum_{p=1}^{6} \bar{J}_\ell^p A_\ell^p + \Sigma_\ell^r \bar{\phi}_\ell V_\ell \;=\; \bar{Q}_\ell V_\ell \tag{2.9}$$

where the cell-averaged values of the flux and multigroup source terms are defined by

$$\bar{\phi}_\ell \equiv \frac{1}{V_\ell} \int_{r\in R_\ell} d^3r\ \phi_\ell(\underline{r}) \tag{2.10}$$

and

$$\bar{Q}_\ell \equiv \frac{1}{V_\ell} \int_{r\in R_\ell} d^3r\ Q_\ell(\underline{r}). \tag{2.11}$$

$\bar{J}_\ell^p$, the surface-averaged component of the net current in direction $\hat{n}_p$ at surface A_ℓ^p is defined by

$$\bar{J}_\ell^p \equiv -\frac{1}{A_\ell^p} \int_{A_\ell^p} dA_\ell^p\ \hat{n}_p\cdot\underline{\nabla}\phi_\ell(\underline{r}). \tag{2.12}$$

The solution of Eq. (2.9) clearly requires additional relationships between the leakages and the cell-averaged fluxes in R_ℓ and its six neighbors. Such relationships are obtained by assuming:

(1) the flux varies linearly from the center of the mesh cell to the midpoints of any of its six surfaces;

(2) along each surface, A_ℓ^p, variations in the normal derivative to the surface may be neglected.

These assumptions are equivalent to introducing a multidimensional Taylor series expansion of the flux about the cell midpoint and truncating terms of $O(h^2)$ and higher.[20]

Application of assumptions (1) and (2) to Eq. (2.10), Eq. (2.11) and Eq. (2.12) lead to the following approximations:

$$\bar{\phi}_\ell \cong \phi_\ell \equiv \phi_\ell(0,0,0), \tag{2.13}$$

$$\bar{Q}_\ell \cong Q_\ell \equiv Q_\ell(0,0,0), \tag{2.14}$$

$$\bar{J}^p_\ell \cong J^p_\ell \equiv \begin{cases} -J^x_\ell(-\Delta x_i/2) & p = 1 \qquad (2.15a) \\ J^x_\ell(\Delta x_i/2) & p = 2 \qquad (2.15b) \end{cases}$$

where

$$J^x_\ell(\Delta x_i/2) \equiv J^x_\ell(\Delta x_i/2,0,0) = -D_\ell \frac{\partial \phi_\ell}{\partial x}(x,0,0)\Big|_{x = \Delta x_i/2}. \tag{2.16}$$

Similar equations hold for the remaining directions y (p = 3 or 4) and z (p = 5 or 6). The derivative in Eq. (2.16) is approximated by using assumption (1). We obtain the following expression for the component of the net current in direction x at the boundary of cell R_ℓ:

$$J^x_\ell(\Delta x_i/2) \cong -D_\ell \frac{\phi_\ell(\Delta x_i/2,0,0) - \phi_\ell}{\Delta x_i/2} \tag{2.17}$$

Evaluating and equating two expressions for the x-directed current component across the interface between cells R_ℓ and R_m (e.g. $J^x_\ell(\Delta x_i/2)$ and $J^x_m(-\Delta x_{i+1}/2)$) and then applying the interface conditions, Eq. (2.3) and Eq. (2.4), leads to the following expression for the interface flux

$$\phi_\ell(\Delta x_i/2,0,0) = \frac{D_\ell/\Delta x_i}{D_\ell/\Delta x_i + D_m/\Delta x_{i+1}} \phi_\ell + \frac{D_m/\Delta x_{i+1}}{D_\ell/\Delta x_i + D_m/\Delta x_{i+1}} \phi_m \tag{2.18}$$

Substitution of Eq. (2.18) into Eq. (2.17) leads to the desired expression for the net current component:

$$J^x_\ell(\Delta x_i/2) = \gamma^x_{\ell m}(\phi_\ell - \phi_m) \tag{2.19a}$$

or

$$J^x_m(-\Delta x_{i+1}/2) = -\gamma^x_{m\ell}(\phi_m - \phi_\ell) \tag{2.19b}$$

where

$$\gamma^x_{\ell m} = \gamma^x_{m\ell} \equiv \frac{1}{\frac{\Delta x_i}{2D_\ell} + \frac{\Delta x_{i+1}}{2D_m}} \tag{2.20}$$

Similar equations are obtained for directions y and z.

When $\Delta x_i/2$ corresponds to an external boundary in cell R_ℓ or if cell $R_m = R_{i+1jk}$ is a blackness theory region, then Eq. (2.5) provides the relation needed for determining the boundary coupling coefficient $\gamma^x_{\ell b} \equiv \gamma^x_{\ell m}$. Rewriting Eq. (2.5) in terms of the net current we obtain

$$\pm J^x_\ell(\pm\Delta x_i/2) = \left(\frac{\beta}{\alpha}\right)\phi_\ell(\pm\Delta x_i/2,0,0). \tag{2.21}$$

The flux at the cell boundary is obtained by eliminating $J^x_\ell(\pm\Delta x_i/2)$ from Eq. (2.17) and Eq. (2.21), and solving for $\phi_\ell(\pm\Delta x_i/2,0,0)$:

$$\phi_\ell(\pm\Delta x_i/2,0,0) = \frac{D_\ell/\Delta x_i}{D_\ell/\Delta x_i + (\beta/\alpha)/2}\,\phi_\ell. \tag{2.22}$$

The general expression for the leakage term at the boundary is obtained by substituting Eq. (2.22) into Eq. (2.21), e.g.

$$\left.\begin{aligned} J^x_\ell(\Delta x_i/2) &= \gamma^x_{\ell b}\phi_\ell \\ J^x_\ell(-\Delta x_i/2) &= -\gamma^x_{b\ell}\phi_\ell \end{aligned}\right\} \tag{2.23}$$

where

$$\gamma^x_{\ell b} = \gamma^x_{b\ell} \equiv \frac{1}{\frac{\Delta x_i}{2D_\ell}}\frac{1}{+\frac{1}{(\beta/\alpha)}}. \tag{2.24a}$$

Rearrangement of terms β and α permit evaluation of Eq. (2.24a) when $\alpha = 0$ or $\beta = 0$, i.e.

$$\gamma^x_{\ell b} \equiv \frac{2\beta D_\ell}{\beta\Delta x_i + 2\alpha D_\ell}. \tag{2.24b}$$

Equation (2.13), Eq. (2.14), Eq. (2.19) and Eq. (2.23) can now be combined to form the mesh-centered finite difference approximation to Eq. (2.9), i.e.

$$-\sum_{\substack{p=1 \\ m_p \neq b}}^{6} a_{\ell m_p} \phi_{m_p} + b_\ell \phi_\ell = q_\ell \tag{2.25}$$

where R_{m_p} is the cell adjacent to R_ℓ at surface A_ℓ^p and

$$a_{\ell m_p} = A_\ell^p \gamma_{\ell m_p}^s \tag{2.26}$$

$$b_\ell = \Sigma_\ell^r V_\ell + \sum_{p=1}^{6} a_{\ell m_p} \tag{2.27}$$

$$q_\ell = Q_\ell V_\ell . \tag{2.28}$$

2.1.3 Comments Regarding All Geometry Options

The terms $\gamma_{\ell m}^s$ and the formulas for calculating the indices m_p of the P cells R_{m_p} adjacent to R_ℓ are tabulated in Table 2.1 for all geometry options in DIF3D. Table 2.2 tabulates the corresponding area and volume elements that are illustrated in Figs. 2.1-2.3. Not included here are the two- and three-dimensional hexogonal geometry options associated with the DIF3D nodal option.[5]

Mesh cell numbering proceeds in a point by point, row by row and plane by plane fashion for both orthogonal and triangular geometries. Figures 2.4-2.6 illustrate the mesh cell numbering for the two basic triangular geometry options (i.e. parallelogram or rectangular boundary domains). Including alternately upward and downward pointing triangles in a single row, permits the same data structure to be used for both rectangular and triangular geometry.

The periodic boundary conditions offered by DIF3D are limited. The opposite face periodicity option, models a repeating lattice in the "X"-direction in orthogonal geometries (i.e. R_{Ijk} is coupled to R_{1jk}). The periodic coupling in the Θ-direction of Θ-R-Z geometry also fits this model.

The rotational periodicity option applies to only the lower x- and lower y-face combination which intersect at the origin in either the orthogonal or the triangular (parallelogram boundary domain only) geometry options. This option models the case in which the A_ℓ^3 surface of cells R_{ilk} are connected to the A_m^1 surface of R_{1jk} where

Table 2.1 Mesh-Centered Finite-Difference Formulas

	Orthogonal	Triangular[a]
Geometry Option[b]:	X, XY, XYZ R, RZ, ΘR, ΘRZ	T, TZ
$\gamma^s_{\ell m}$:	$\dfrac{1}{\dfrac{\Delta s_\ell}{2D_\ell} + \dfrac{\Delta s_m}{2D_m}}$	$\dfrac{1}{\dfrac{\Delta s_\ell}{3D_\ell} + \dfrac{\Delta s_m}{3D_m}}$
$\gamma^s_{\ell b}$:	$\dfrac{1}{\dfrac{\Delta s_\ell}{2D_\ell} + \dfrac{1}{(\beta/\alpha)}}$	$\dfrac{1}{\dfrac{\Delta s_\ell}{3D_\ell} + \dfrac{1}{(\beta/\alpha)}}$
Δs^c_ℓ : $(s_{\ell+1} - s_\ell)$	$\begin{cases} 1 & s_\ell \neq \Theta_i \\ \dfrac{r_{j+1} + r_j}{2} & s_\ell = \Theta_i \end{cases}$	$\sqrt{3}\Delta x$
p = 1 or 2[d]:	$m_p = (i \mp 1, j, k)$	$m_p = (i \mp 1, j, k)$
p = 3 or 4[d]:	$m_p = (i, j \mp 1, k)$	$m_p = (i \mp \delta, j \mp 1, k)$[e]
p = 5 or 6[d]:	$m_p = (i, j, k \mp 1)$	-

[a] Axial (z-direction) formulas in TZ geometry are identical to the orthogonal case.

[b] Coordinates are ordered as listed (e.g. ΘRZ implies "X"=Θ, "Y"=R and "Z"=Z.

[c] $\sqrt{3}\Delta x$ is triangle height or 1/2 hex pitch, ($2\Delta x \equiv$ triangle side length).

[d] Sign convention for $m \equiv m_p$: odd numbered p take minus (−) sign, even numbered p take plus (+) sign.

[e] Triangular geometry offset index:

$$\delta = \begin{cases} -1 & \text{parallelogram boundary domain, 60° symmetry,} \\ 0 & \text{rectangular boundary domain,} \\ 1 & \text{parallelogram boundary domain, 120° symmetry.} \end{cases}$$

Table 2.2 Areas and Volumes for Each Geometry Option[a]

Geometry	$A^1_\ell = A^x_{ijk}$ $i=1,2,\ldots,I+1$	$A^3_\ell = A^y_{ijk}$ $j=1,2,\ldots,J+1$	$A^5_\ell = A^z_{ijk}$ $K=1,2,\ldots,K+1$	V_{ijk}
X	1			Δx_i
XY	Δy_j	Δx_i		$\Delta x_i \Delta y_j$
XYZ	$\Delta y_j \Delta z_k$	$\Delta x_i \Delta z_k$	$\Delta x_i \Delta y_j$	$\Delta x_i \Delta y_j \Delta z_k$
R	$2\pi r_i$			$(r^2_{i+1}-r^2_i)\pi$
RZ	$2\pi r_i \Delta z_j$	$\pi(r^2_{i+1}-r^2_i)$		$(r^2_{i+1}-r^2_i)\pi\Delta z_j$
ΘR	Δr_j	$r_j \Delta\Theta_i$		$\frac{1}{2}(r^2_{j+1}-r^2_j)\Delta\Theta_i$
ΘRZ	$\Delta r_j \Delta z_k$	$r_j \Delta\Theta_i \Delta z_k$	$\frac{1}{2}(r^2_{j+1}-r^2_j)\Delta\Theta_i$	$\frac{1}{2}(r^2_{j+1}-r^2_j)\Delta\Theta_i \Delta z_k$
T^{bc}	$2\Delta x$	$\eta(t)2\Delta x$		$\sqrt{3}\,\Delta x^2$
TZ^{bc}	$2\Delta x \Delta z_k$	$\eta(t)2\Delta x \Delta z_k$	$\sqrt{3}\,\Delta x^2$	$\sqrt{3}\,\Delta x^2 \Delta z_k$
T^{bd}	$\mu(i)2\Delta x$	$\eta(t+j-1)\xi(i)2\Delta x$		$\xi(i)\sqrt{3}\,\Delta x^2$
TZ^{bd}	$\mu(i)2\Delta x \Delta z_k$	$\eta(t+j-1)\xi(i)2\Delta x \Delta z_k$	$\xi(i)\sqrt{3}\,\Delta x^2$	$\xi(i)\sqrt{3}\,\Delta x^2 \Delta z_k$

[a] Unless otherwise noted, indices (i,j,k) take the values i=1,2,...,I, j=1,2,...,J and k=1,2,...K. Note that $A^{p+1}_{m_p} = A^p_\ell$, p = 1,3,5 where m_p is given in Table 2.1.

[b] "T" denotes the triangular geometry option. $\eta(t) = \text{mod}(t,2)$ accounts for the fact that alternate "y-direction" surface areas are non-existant.

[c] Parallelogram domain boundary option with 60° (t = 1) or 120°(t = i+1) symmetry.

[d] Rectangular domain boundary option with 90° symmetry (t = i+1), 180° symmetry (t = i+NTHPT) or full core option (m = i+NTHPT) where NTHPT = (1 or 2) is defined in the GEODST description (Appendix C). The functions $\mu(i) = \begin{cases} 1 & 1<i<I+1 \\ \sqrt{3/2} & i=1 \text{ or } i=I+1 \end{cases}$ and $\xi(i) = \begin{cases} 1 & 1<i<I+1 \\ 1/2 & i=1 \text{ or } i=I+1 \end{cases}$ account for the fact that R_{1jk} and R_{Ijk} are always half triangles.

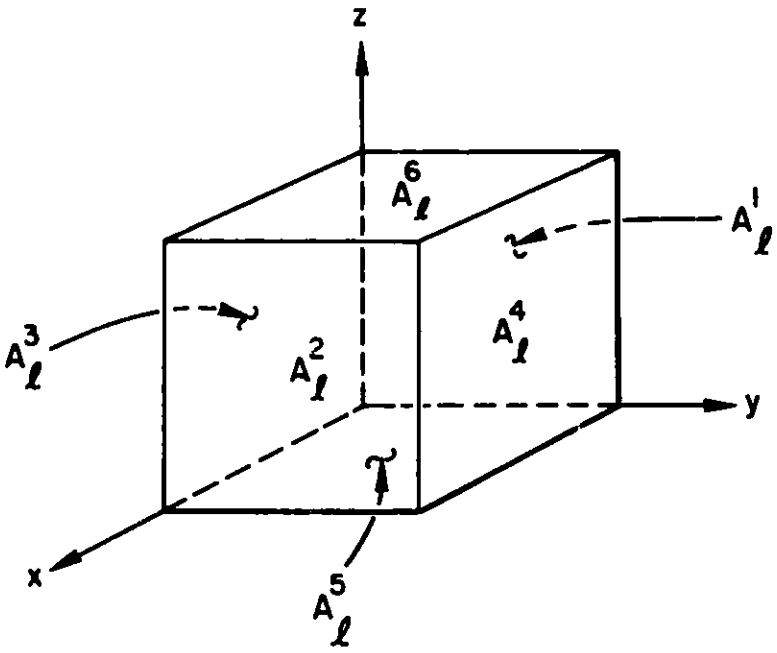

Fig. 2.1. X-Y-Z Volume Element

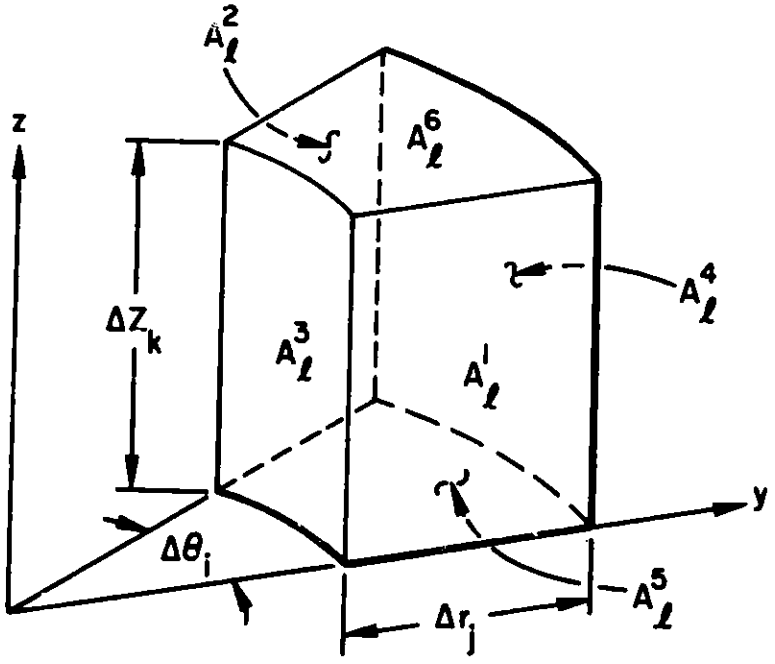

Fig. 2.2. θ-R-Z Volume Element

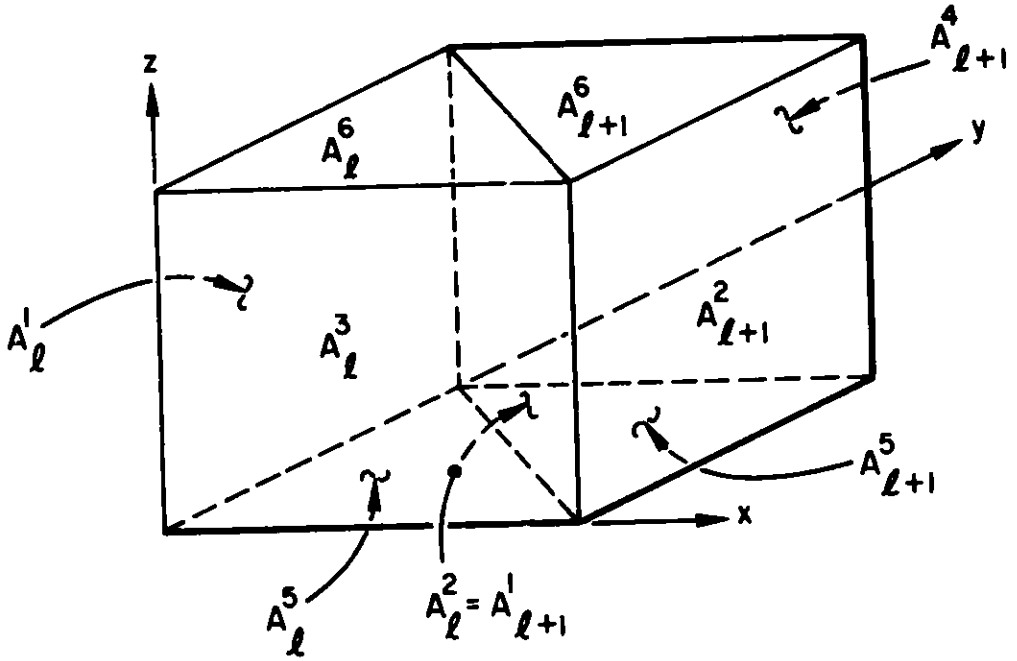

Fig. 2.3. Triangular-Z Volume Elements

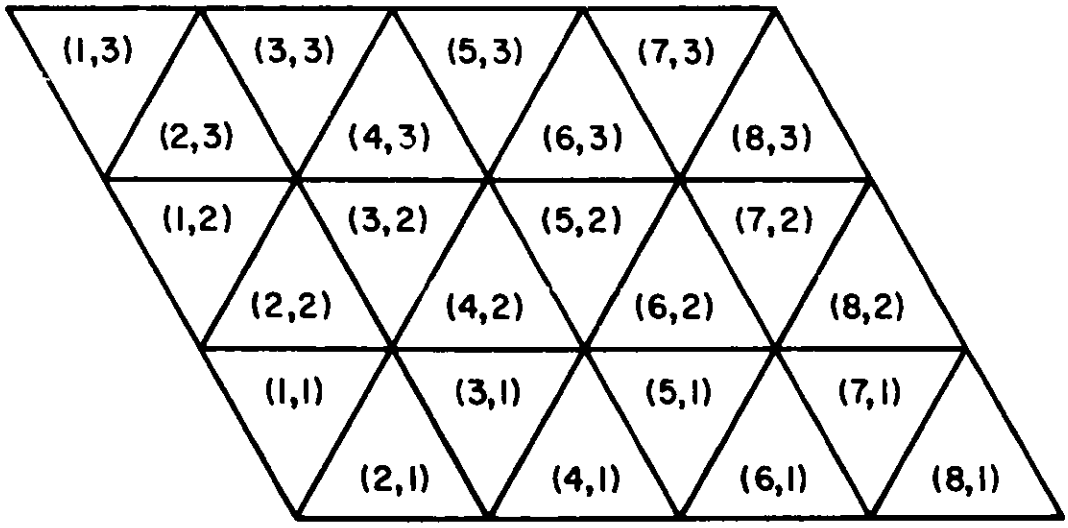

Fig. 2.4. Parallelogram Boundary Domain (120° planar symmetry)

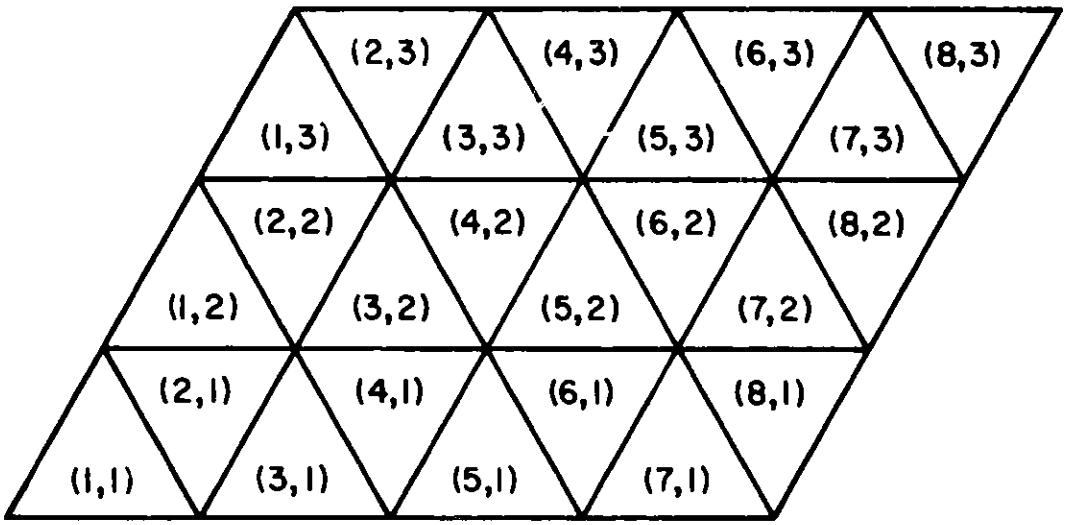

Fig. 2.5. Parallelogram Boundary Domain (60° planar symmetry)

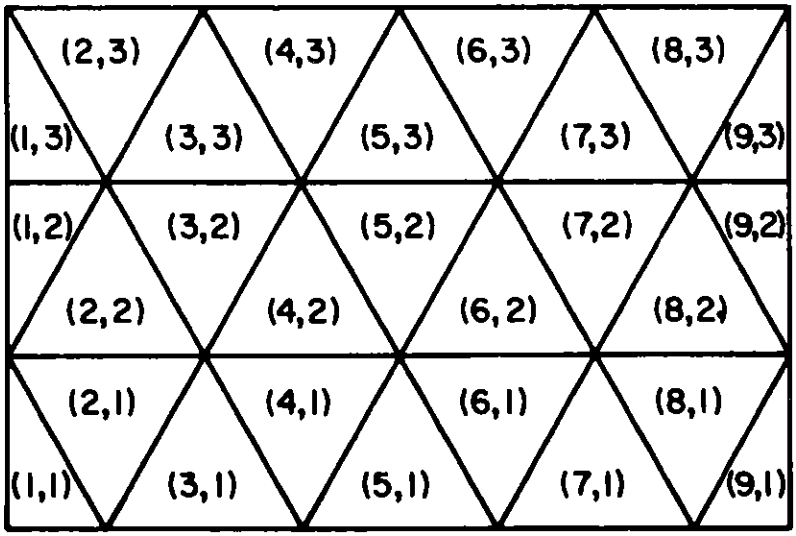

Fig. 2.6. Rectangular Boundary Domain (90°, 180° or 360° planar symmetry)

$j=i$, $i=1,2,\ldots,I$ in orthogonal geometry;

$j=(i+1)/2$, $i=1,3,5,\ldots$ in triangular geometry (60° symmetry);

$j=i/2$, $i=2,4,6,\ldots$ in triangular geometry (120° symmetry).

Conversely, cells R_{ijk} are connected to R_{i1k} where

$i=j$, $j=1,2,\ldots,J$ in orthogonal geometry;

$i=2j-1$, $j=1,2,\ldots,J$ in triangular geometry (60° symmetry);

$i=2j$, $j=1,2,\ldots,J$ in triangular geometry (120° symmetry).

2.1.4 The Matrix Equations and Their Properties

The mesh-centered finite-difference equations (Eq. (2.25) in eigenvalue form) for the cell-averaged fluxes can be written in matrix form as

$$([D_g] + [\Sigma_g])\underline{\phi}_g - \sum_{g' \neq g} [T_{gg'}]\underline{\phi}_{g'} = \frac{1}{\lambda} [\chi_g] \sum_{g'=1}^{G} [F_{g'}]\underline{\phi}_{g'} \tag{2.29}$$

where $\underline{\phi}_g$ is the N-dimensional vector of (approximate) fluxes on the finite difference mesh. The matrices $[\Sigma_g]$, $[T_{gg'}]$, $[F_g]$ and $[\chi_g]$ are N×N diagonal matrices defined by

$$[\Sigma_g] = \text{diag}\,(\Sigma_\ell^{r,g} V_\ell) \tag{2.30}$$

$$[T_{gg'}] = \text{diag}\,(\Sigma_\ell^{s,gg'} V_\ell) \tag{2.31}$$

$$[F_g] = \text{diag}\,(\nu\Sigma_\ell^{f,g} V_\ell) \tag{2.32}$$

$$[\chi_g] = \text{diag}\,(\chi_\ell^g) \tag{2.33}$$

where N is the number of cells in the finite-difference mesh. The unknowns in $\underline{\phi}_g$ are ordered in a linear fashion, row by row and plane by plane. Given this linear ordering, the N×N matrix $[D_g]$ contains three, five or seven nonzero stripes for one-, two- or three-dimensional geometries, respectively. It operates on $\underline{\phi}_g$ to yield the net leakage across the faces of each mesh cell.

The G Eqs. (2.29) can be condensed into the single matrix equation

$$[M]\underline{\Phi} = \frac{1}{\lambda}[B]\underline{\Phi}. \tag{2.34}$$

where [M] and [B] are square and of order N*G and $\underline{\Phi}$ = col $[\underline{\Phi}_1, \underline{\Phi}_2, \ldots, \underline{\Phi}_G]$. The matrix [M] is given by

$$[M] = \begin{bmatrix} [A_1] & & & [0] \\ & [A_2] & & \\ & & \ddots & \\ [0] & & & [A_G] \end{bmatrix} + \begin{bmatrix} [0] & [T_{12}] & \cdots & [T_{1G}] \\ [T_{21}] & [0] & & \vdots \\ \vdots & & \ddots & [T_{G,G-1}] \\ [T_{G1}] & [T_{G2}] & [T_{G,G-1}] & [0] \end{bmatrix} \tag{2.35}$$

where $[A_g]$ ($\equiv [D_g] + [\Sigma_g]$) is the leakage-plus-removal matrix operator and [0] is the null matrix. As shown in Eq. (2.35), the in-group scatter term is ignored in DIF3D. The symmetric matrix A_g is defined by

$$[A_g] = \begin{bmatrix} \ddots & \ddots & & \ddots & \\ [A^{gx}_{J-1k}] & [A^{gy}_{Jk}] & & [A^{gz}_{J-1k+1}] & \\ & [A^{gx}_{Jk}] & [0] & & [A^{gz}_{Jk+1}] \\ \text{(symmetric)} & & [A^{gx}_{1k+1}] & [A^{gy}_{2k+1}] & [A^{gz}_{1k+2}] \\ & & \ddots & \ddots & \ddots \end{bmatrix} \tag{2.36}$$

where the submatrices in Eq. (2.36) are defined in terms of coefficients $a^s_{ijk} = a_{\ell m_p}$, p=1,3 or 5 and $b_{ijk} = b_\ell$ from Eqs. (2.26) and (2.27):

$$A^{gy}_{jk} = \begin{bmatrix} b_1 & -a^x_2 & & & & \\ -a^x_2 & b_2 & -a^x_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & -a^x_{I-1} & b_{I-1} & -a^x_I \\ & & & & -a^x_I & b_I \end{bmatrix}_{jkg} \tag{2.37}$$

$$[A^{gy}_{jk}] = \text{diag}\,(a^y_i)_{jkg} \tag{2.38}$$

$$[A^{gz}_{jk}] = \text{diag}\,(a^{z}_{i})_{jkg}. \tag{2.39}$$

By defining the N*G by N matrices

$$[F] = \text{col}\left[[F_1], [F_2], \ldots, [F_G]\right] \tag{2.40}$$

and

$$[\chi] = \text{col}\left[[\chi_1], [\chi_2], \ldots, [\chi_G]\right], \tag{2.41}$$

the matrix [B] can be written as

$$[B] = [\chi][F]^{T}, \tag{2.42}$$

where T denotes the transpose of a matrix.

The matrices used in Eqs. (2.34)-(2.42) possess a number of properties which provide a sound theoretical basis for the iteration methods which are discussed in Sec. 2.2. For any physically realistic set of assumptions, the diagonal matrices $[T_{gg'}]$, $[\chi_g]$ and $[F_g]$ are non-negative matrices. It has been shown[21] that the matrices $[A_g]$ are irreducible Stieltjes matrices and that the inverse of each $[A_g]$ has all positive entries, i.e., $[A_g]^{-1}>0$. Because of these properties, the matrix [M] is nonsingular[22] and the eigenvalue problem Eq. (2.34) can be written as

$$\lambda\,\underline{\Phi} = [M]^{-1}[B]\,\underline{\Phi}. \tag{2.43}$$

Under quite general conditions, Froehlich[23] has shown that Eq. (2.43) has a unique positive eigenvector $\underline{\Phi}_0$ and a corresponding single positive eigenvalue λ_0 greater than the absolute value of any other eigenvalue of Eq. (2.43). Furthermore any positive eigenvector of $[M]^{-1}[B]$ is a scalar multiple of $[\underline{\Phi}]$.

The properties of [B] permit a reduction of the matrix eigenvalue problem which must be solved to obtain λ_0 from one of order N*G (Eq. (2.43)) to one of only order N.[12] Advantage is taken of this fact in obtaining the outer iteration method presented in Sec. 2.2 which is used to obtain λ_0 and $\underline{\Phi}_0$. This reduction is accomplished by first noting that $[M]^{-1}[B]$ is of order N*G and therefore has N*G eigenvalues. However, the rank of [F] is only N, thus making the rank of $[M]^{-1}[B]$ only N. Hence, (G-1)*N of its eigenvalues are zero. The nonzero eigenvalues can be determined by considering the reduced but equivalent problem of order N.

Following Ref. 12, but considering a full scattering matrix, this reduction is accomplished by first defining the fission source vector, $\underline{\Psi}$, as

$$\underline{\Psi} \equiv [F]^{T}\,\underline{\Phi} = \sum_{g=1}^{G} [F_g]\,\underline{\Phi}_g \tag{2.44}$$

and the N*G × N matrix [L] as

$$[L] = \text{col}\,[L_1], [L_2], \ldots, [L_G] = [M]^{-1}[\chi], \tag{2.45}$$

where the N × N matrices $[L_g]$ are defined as

$$[L_g] \equiv [A_g]([\chi_g] + \sum_{g' \neq g} [T_{gg'}][L_{g'}]). \tag{2.46}$$

These definitions plus Eq. (2.34) permit the group g flux vector $\underline{\phi}_g$, to be written as

$$\underline{\phi}_g = \frac{1}{\lambda}[L_g]\underline{\psi}. \tag{2.47}$$

Premultiplying Eq. (2.43) by $[F]^T$ and using Eqs. (2.42) and (2.44) yields the reduced problem

$$\lambda\underline{\psi} = [Q]\underline{\psi}, \tag{2.48}$$

where

$$[Q] = [F]^T[L] = \sum_{g=1}^{G} [F_g][L_g]. \tag{2.49}$$

If $\underline{\phi}$ and λ are an eigenvector and corresponding nonzero eigenvalue of $[M]^{-1}[B]$, then $\underline{\psi}$ and λ must be an eigenvector and eigenvalue of [Q] and vice versa. Furthermore, by making use of a similarity transformation, it has been shown[12] that the nonzero eigenvalue spectrum of [Q] is identical to the nonzero spectrum of $[M]^{-1}[B]$ and that any non-negative eigenvector of [Q] is either a scalar multiple of $\underline{\psi}_0$ or else corresponds to a zero eigenvalue, where $\underline{\psi}_0$ corresponds to λ_0. Thus the two eigenvalue problems, Eq. (2.43) and Eq. (2.48), are equivalent.

2.2 Solution Strategies

The finite-difference equations are solved by the well-known fission source iteration method[24] accelerated by the Chebyshev semi-iterative method.[25,26] At each fission source (or "outer") iteration, the vector of neutron fluxes for each group is computed by solving the finite-difference equations with a known group-dependent source term. This solution is accomplished via sucessive sweeps through the spatial mesh. Each such inner iteration sweep iteratively inverts the leakage-plus-removal matrix operator using the line-successive-overelaxation procedure.[27]

The acceleration strategies for DIF3D are linear, well-founded and proven, and they relieve users of the burden of specifying optimum parameters for large classes of reactor models. Theoretical aspects of the two acceleration methods are presented in Sections 2.2.1 and 2.2.2, respectively. Computational and data management aspects of each method are described in Sections 2.2.3-2.2.5. The adjoint problem is discussed in Section 2.2.6. Problems with upscattering are solved using the iteration strategy reported in Section 2.2.7. Section 2.2.8 describes aspects of the inhomogeneous problem.

2.2.1 The Chebyshev Accelerated Outer (Fission Source) Iterations

The outer iterations seek to determine the fundamental eigenvector, $\underline{\psi}_0$, and corresponding eigenvalue, λ_0, of Eq. (2.48) or the fundamental eigenvector, $\underline{\phi}_0$, and λ_0 of Eq. (2.43). Most few-group codes, such as PDQ-7, treat the flux problem, Eq. (2.43). This is due to two factors. First, most thermal power reactors of interest have large reflecting regions which contain no fissionable materials. For any outer iteration method which utilizes an outer iteration acceleration procedure such as the one described in this report, acceleration of the fission source does not markedly improve acceleration of the solution in these reflecting regions unless much additional effort is invested in the inner iterations. This point is elaborated in Sec. 2.2.4. Second, for the two to four energy group structures which are typically used for thermal reactor calculations, the data storage and transfer requirements associated with acceleration procedures based on the fluxes are not prohibitively larger than if the fission source were used.

In fast reactors, on the other hand, the data management requirements associated with accelerating the flux vector are at least an order of magnitude greater than those associated with the fission source for the ten to thirty energy groups which are typically used for fast reactor calculation. In addition, the fast reactor cores under consideration at the time of DIF3D's development tended to be more tightly coupled with relatively small non-fissionable regions. Consequently, the cost of the increased number of outer iterations resulting from the fission source acceleration is more than compensated by the savings in I/O resources. These conclusions are borne out by the numerical results presented in Ref. (1). Later, application to large-scale heterogeneous fast reactor core designs[28] also proved highly efficient.

In the method reported here, approximations to λ_0 and $\underline{\psi}_0$, the fundamental eigenvalue and eigenvector of [Q], are obtained by the well-known power iteration method. It is assumed that the eigenvalue spectrum of [Q] satisfies $\lambda_0 > |\lambda_1| > |\lambda_2| > \ldots > |\lambda_{N-1}|$ and that $\underline{\psi}_1$ is the eigenvector associated with λ_1. The power method proceeds as

$$\underline{\psi}^{(n)} = \frac{1}{\lambda^{(n-1)}} [Q]\underline{\psi}^{(n-1)} \tag{2.50a}$$

and

$$\lambda^{(n)} = \lambda^{(n-1)} \frac{\|\underline{\psi}^{(n)}\|_1}{\|\underline{\psi}^{(n-1)}\|_1}, \tag{2.50b}$$

where n is the outer iteration index and $\|\cdot\|_1$ denotes the L_1 norm. The actual computation of the product $[Q]\underline{\psi}^{(n-1)}$ in Eq. (2.50a) involves another level of iteration, the inner iteration, and is discussed in the next section. A later section describes a third level of iteration, the upscatter iteration which occurs outside the inner iteration for all groups when upscattering source terms are present.

Because the largest (in modulus) eigenvalue of [Q] is real and simple, the power method is guaranteed to converge for any arbitrary non-negative initial vector $\underline{\psi}^{(0)}$ to λ_0 and $c\underline{\psi}_0$, where c is some positive constant. If it is assumed that the eigenvalue estimates $\lambda^{(n)}$ are sufficiently well converged to λ_0 and that $\underline{\psi}^{(0)}$ can be expanded in terms of the $\underline{\psi}_i$, the eigenvectors of [Q], then the rate at which $\underline{\psi}^{(n)}$ converges to $\underline{\psi}_0$ depends on the separation of λ_0 from the other eigenvalues of [Q].[12] This convergence rate depends on the dominance ratio, $\bar{\sigma}$, given by

$$\bar{\sigma} = \max_{i \neq 0} \frac{|\lambda_i|}{\lambda_0} , \tag{2.51}$$

with the convergence rate ultimately being controlled by $(\bar{\sigma})^n$.

The dominance ratios of large thermal power reactors typically are of the order of 0.95 or larger, implying relatively slow convergence of the iterative process given by Eq. (2.50). This fact led to the search for methods to accelerate this convergence for thermal reactor codes, of which the acceleration method based on Chebyshev polynomials used by PDQ-7[12,13] and the class of methods known as coarse-mesh rebalance[23,24] methods are the best known. Dominance ratios for large heterogeneous fast reactors can also be as large as 0.95. In addition, typical fast reactor multigroup energy structures are characterized by nearly full downscattering matrices. The group-by-group calculation of the scattering source required for each outer iteration becomes a costly, input/output-bound calculation when such energy structures are used in large multidimensional calculations. Both of these factors motivate the use of an efficient outer iteration acceleration technique in fast reactor diffusion theory calculations.

A Chebyshev acceleration strategy similar to that used in PDQ-7 is utilized in the solution method presented here. The primary difference is that while PDQ-7 accelerates the flux vector, $\underline{\Phi}$, DIF3D accelerates the fission source, $\underline{\psi}$. The motivations for this have been presented above. Its application is based on the assumptions that the eigenvalues of [Q] are real and non-negative and are ordered as $\lambda_0 > \lambda_1 > \lambda_2 > \ldots > \lambda_{N-1} > 0$ and that the eigenvectors $\underline{\psi}_i$ of [Q] form a basis for the N-dimensional vector space. Following the derivations in Refs. 12 and 13, the basic power iteration is accelerated by choosing a linear combination of the eigenvector iterates $\underline{\psi}^{(n)}$ such that

$$\tilde{\underline{\psi}}^{(n^*+p)} = \sum_{j=0}^{p} a_{jp} \underline{\psi}^{(n^*+j)} , \tag{2.52}$$

where n* is the outer index where this acceleration begins and p successive fission source iterates are employed. The objective is to choose the coefficients such that $\tilde{\underline{\psi}}^{(n^*+p)}$ approximates $\underline{\psi}_0$ more closely than does $\underline{\psi}^{(n^*+p)}$.

Based on the assumption of completeness, $\underline{\psi}^{(n^*)}$ can be written as

$$\underline{\psi}^{(n^*)} = \sum_{i=0}^{N-1} c_i \underline{\psi}_i . \tag{2.53}$$

For a sufficiently converged eigenvalue estimate $\underline{\lambda}^{(n^*)}$, Eqs. (2.50a) and (2.53) imply that Eq. (2.52) can be written as

$$\underline{\tilde{\psi}}^{(n^*+p)} \approx \sum_{i=0}^{N-1} c_i \sum_{j=0}^{p} a_{jp} \left(\frac{\lambda_i}{\lambda_0}\right)^p \underline{\psi}_i . \tag{2.54}$$

Letting $P_p(x) \equiv \sum_{j=0}^{p} a_{jp} x^p$, Eq. (2.54) becomes

$$\underline{\tilde{\psi}}^{(n^*+p)} \approx P_p\left(\frac{1}{\lambda_0}[Q]\right) \underline{\psi}^{(n^*)} = c_0 P_p(1) \underline{\psi}_0 + \sum_{i=1}^{N-1} c_i P_p \left(\frac{\lambda_i}{\lambda_0}\right) \underline{\psi}_i . \tag{2.55}$$

The sum on the R.H.S. of Eq. (2.55) is the error. This error is minimized in a practical sense by choosing $P_p(x)$ such that $P_p(1)=1$ and $\max_{0 \le x \le \bar{\sigma}} P_p(x)$ is minimized. This is accomplished by choosing $P_p(x)$ in terms of Chebyshev polynomials as[25]

$$P_p(x) = \frac{C_p\left(\frac{2x}{\bar{\sigma}} - 1\right)}{C_p\left(\frac{2}{\bar{\sigma}} - 1\right)}, \tag{2.56}$$

where the $C_p(y) = \cosh(p \cosh^{-1} y)$, $y > 1$. Given the well known recurrence relationships for Chebyshev polynomials, the recursion relationship for $P_p(x)$ is

$$P_{p+1}(x) = 2\left(\frac{2x}{\sigma} - 1\right) \left(\frac{\cosh[p\gamma]}{\cosh[(p+1)\gamma]}\right) P_p(x) - \left(\frac{\cosh[(p-1)\gamma]}{\cosh[(p+1)\gamma]}\right) P_{p-1}(x), \quad p > 1, \tag{2.57}$$

where

$$P_0(x) = 1,$$

$$P_1(x) = \frac{\left(\frac{2x}{\bar{\sigma}} - 1\right)}{\left(\frac{2}{\bar{\sigma}} - 1\right)}, \tag{2.58}$$

and

$$\gamma = \cosh^{-1}\left(\frac{2}{\bar{\sigma}} - 1\right). \tag{2.59}$$

This leads to the accelerated iterative procedure for $p \geq 1$:

$$\underline{\psi}^{(n^*+p)} = \frac{1}{\lambda^{(n^*+p-1)}} [Q]\tilde{\underline{\psi}}^{(n^*+p-1)}, \tag{2.60a}$$

$$\tilde{\underline{\psi}}^{(n^*+p)} = \tilde{\underline{\psi}}^{(n^*+p-1)} + \alpha_p[\underline{\psi}^{(n^*+p)} - \tilde{\underline{\psi}}^{(n^*+p-1)}]$$

$$+ \beta_p[\tilde{\underline{\psi}}^{(n^*+p-1)} - \tilde{\underline{\psi}}^{(n^*+p-2)}], \tag{2.60b}$$

$$\lambda^{(n^*+p)} = \lambda^{(n^*+p-1)} \frac{\| \tilde{\underline{\psi}}^{(n^*+p)} \|_1}{\| \tilde{\underline{\psi}}^{(n^*+p-1)} \|_1}, \tag{2.60c}$$

where

$$\alpha_1 = \frac{2}{2-\bar{\sigma}}, \quad \beta_1 = 0,$$

$$\alpha_p = \frac{4}{\bar{\sigma}} \left(\frac{\cosh[(p-1)\gamma]}{\cosh[p\gamma]}\right), \tag{2.61}$$

$$\beta_p = \left(1 - \frac{\bar{\sigma}}{2}\right)\alpha_p - 1.$$

To apply the iteration schemes given by Eqs. (2.50) and (2.60), the dominance ratio $\bar{\sigma}$ must be obtained and a suitable convergence criterion must be applied to measure convergence. It has been shown[21] that if $\underline{\psi}^{(0)}$ is a non-negative vector, then $\lim_{n\to\infty} \lambda^{(n)} = \lambda_0$ and $\lim_{n\to\infty} \underline{\psi}^{(n)} = c\underline{\psi}_0$. In addition, if the i-th components of $\underline{\psi}^{(n-1)}$ and $\underline{\psi}^{(n)}$ are written as $\psi_i^{(n-1)}$ and $\psi_i^{(n)}$ and if $\bar{\lambda}^{(n)}$ and $\underline{\lambda}^{(n)}$ are defined as

$$\bar{\lambda}^{(n)} \equiv \max_i \frac{\psi_i^{(n)}}{\psi_i^{(n-1)}} , \quad \underline{\lambda}^{(n)} \equiv \min_i \frac{\psi_i^{(n)}}{\psi_i^{(n-1)}} , \tag{2.62}$$

then

$$\bar{\lambda}^{(n)} \geq \lambda_0 \geq \underline{\lambda}^{(n)} , \quad \bar{\lambda}^{(n)} \geq \lambda^{(n)} \geq \underline{\lambda}^{(n)} , \tag{2.63}$$

and

$$\lim_{n\to\infty} \bar{\lambda}^{(n)} = \lim_{n\to\infty} \underline{\lambda}^{(n)} = \lambda_0 .$$

Thus, $\bar{\lambda}^{(n)}$ and $\underline{\lambda}^{(n)}$ provide upper and lower bounds on the eigenvalue estimate based on the behavior of the cellwise fission source components. Because they are related to the behavior of the individual components, they also provide insight into how well the individual components of $\underline{\psi}^{(n)}$ are converged. By defining the relative point error, $\varepsilon_{pt}^{(n)}$, as

$$\varepsilon_{pt}^{(n)} \equiv \max_i \left| \frac{\psi_i^{(n)} - \psi_{0i}}{\psi_{0i}} \right| \tag{2.64}$$

where ψ_{0i} is the i-th component of ψ_0, the true result, and

$$\varepsilon^{(n)} \equiv \frac{\bar{\lambda}^{(n)} - \underline{\lambda}^{(n)}}{2} , \tag{2.65}$$

it has been shown[13] that, for n sufficiently large, $\varepsilon_{pt}^{(n)}$ is approximately bounded as

$$\frac{\varepsilon^{(n+1)}}{1 - \bar{\sigma} + \varepsilon^{(n+1)}} \lesssim \varepsilon_{pt}^{(n)} \lesssim \frac{2\varepsilon^{(n+1)}}{1 - \bar{\sigma} - 2\varepsilon^{(n+1)}} . \tag{2.66}$$

This relationship provides a measure of maximum relative error in any of the components of $\underline{\psi}^{(n)}$. The precise manner in which this measure is applied to check fission source convergence here is discussed in Sec. 2.2.4.

An estimate of the dominance ratio $\bar{\sigma}$ is required both in the fission source extrapolation process given in Eq. (2.60b) and in Eq. (2.66) above. One such estimate can be determined by defining the error vector $\underline{R}^{(n)}$ as

$$\underline{R}^{(n)} \equiv \underline{\psi}^{(n)} - \underline{\psi}^{(n-1)} \tag{2.67}$$

and the decay rate of the error, $E^{(n)}$, as

$$E^{(n)} = \left[\frac{\langle \underline{R}^{(n)}, \underline{R}^{(n)} \rangle}{\langle \underline{R}^{(n-1)}, \underline{R}^{(n-1)} \rangle} \right]^{1/2}, \tag{2.68}$$

where $\langle , \rangle$ denotes an inner product.

For the power method of iteration,[13]

$$\lim_{n \to \infty} E^{(n)} = \sigma. \tag{2.69}$$

Several key algorithmic details associated with the application of the power iteration and Chebyshev acceleration procedures remain to be discussed. These include (a) determining when to start the first acceleration cycle, (b) obtaining improved estimates of the dominance ratio as the acceleration cycles proceed and (c) determining when to start a new acceleration cycle. These are discussed in Sec. 2.2.3.

2.2.2 The Line Successive Overrelaxation of the Inner Iterations

The inner iterations are required in carrying out the operation $[Q]\underline{\psi}^{(n-1)}$ on the R.H.S. of Eq. (2.50a) and (2.60a). From Eqs. (2.46) and (2.47), $[Q]\underline{\psi}^{(n-1)}$ can be written as

$$[Q]\underline{\psi}^{(n-1)} = \sum_{g=1}^{G} [F_g][L_g]\underline{\psi}^{(n-1)} = \lambda^{(n-1)} \sum_{g=1}^{G} [F_g]\underline{\phi}_g^{(n)}, \tag{2.70}$$

where

$$\underline{\phi}_g^{(n)} \equiv \frac{1}{\lambda^{(n-1)}} [L_g]\underline{\psi}^{(n-1)} \tag{2.71}$$

Given the $\underline{\phi}_g^{(n)}$, $[Q]\underline{\psi}^{(n-1)}$ and hence $\underline{\psi}^{(n)}$ can be easily obtained. The definition of $[L_g]$, Eq. (2.46), defines a series of linear equations

$$[A_g]\underline{\phi}_g^{(n)} = \underline{b}_g^{(n)}, \quad g=1, 2, \ldots, G, \tag{2.72}$$

which can be solved for the group flux vectors $\underline{\phi}_g^{(n)}$.

The source $\underline{b}_g^{(n)}$ is given by (see Eq. (2.112b) for the upscatter problem)

$$\underline{b}_g^{(n)} = \sum_{g'<g} [T_{gg'}]\underline{\phi}_{g'}^{(n)} + \frac{1}{\lambda^{(n-1)}}[\chi_g]\underline{\psi}^{(n-1)}. \tag{2.73}$$

For multidimensional problems, the direct inversion of $[A_g]$ matrices in Eq. (2.72) is not practical. The iterative inversion of $[A_g]$ for each group comprise the inner iterations.

Because of its sound theoretical basis and computational simplicity (see Sec. 2.2.4), the line successive overrelaxation method has been chosen for the solution strategy reported here. The matrix [A] in Eq. (2.72) (dropping the group subscript) is split as[27]

$$[A] = [D] - [E] - [F], \tag{2.74}$$

where [D] contains the diagonal of $[A_g]$ plus those off-diagonal coefficients which represent coupling between cell fluxes in each row, [E] contains those blocks of [A] which lie below the diagonal blocks placed in [D], and [F] contains those blocks which lie above the blocks in [D]. The line successive overrelaxation procedure is then given by

$$\underline{\phi}_g^{(m+1)} = [L_\omega]\underline{\phi}_g^{(m)} + \underline{k}_g, \tag{2.75}$$

where

$$[L_\omega] = ([D] - \omega[E])^{-1}(\omega[F] + (1-\omega)[D]) \tag{2.76}$$

and

$$\underline{k}_g = ([D] - \omega[E])^{-1}\omega\ \underline{b}_g. \tag{2.77}$$

The matrix $[L_\omega]$ is the line successive overrelaxation iteration matrix and ω is the overrelaxation factor; both are group-dependent. Because [A] (for each group) is an irreducible consistently-ordered 2-cyclic Stieltjes matrix for the finite differencing schemes used here, the iteration procedure given by Eq. (2.75) is convergent for $1<\omega<2$.[29] Furthermore, there is an optimum value of ω, say ω_b, for which the convergence is the most rapid. This group-dependent value of ω_b is given by[27]

$$\omega_b = \frac{2}{1 + [1 - \rho([L_1])]^{1/2}}, \tag{2.78}$$

where $\rho([L_1])$ is the spectral radius of $[L_1]$, the associated Gauss-Seidel iteration matrix, which can be obtained from Eq. (2.76) by setting $\omega=1$.

Following the procedure outlined in Ref. 30, the value of ω_b can be determined to arbitrary accuracy because the [A] matrix for each group has the properties listed above. For such matrices, if $\underline{x}^{(0)} > 0$ and if

$$\underline{x}^{(m)} \equiv [L_1]\underline{x}^{(m-1)} \tag{2.79a}$$

and

$$\delta^{(m)} \equiv \frac{\langle \underline{x}^{(m)}, \underline{x}^{(m)} \rangle}{\langle \underline{x}^{(m)}, \underline{x}^{(m-1)} \rangle} , \tag{2.79b}$$

then

$$\lim_{m\to\infty} \delta^{(m)} = \rho([L_1]). \tag{2.80}$$

Furthermore, if $x_i^{(m-1)} \neq 0$ and if

$$\bar{\delta}^{(m)} \equiv \max_i \frac{x_i^{(m)}}{x_i^{(m-1)}} ; \qquad \underline{\delta}^{(m)} \equiv \min_i \frac{x_i^{(m)}}{x_i^{(m-1)}} , \tag{2.81}$$

then

$$\bar{\delta}^{(m)} > \rho([L_1]) > \underline{\delta}^{(m)},$$

$$\bar{\delta}^{(m)} > \delta^{(m)} > \underline{\delta}^{(m)}$$

and

$$\lim_{m\to\infty} \bar{\delta}^{(m)} = \lim_{m\to\infty} \underline{\delta}^{(m)} = \rho([L_1]). \tag{2.82}$$

The spectral radius $\rho([L_1])$ can be computed by carrying out the iteration given by Eq. (2.79a), computing $\delta^{(m)}$, $\bar{\delta}^{(m)}$ and $\underline{\delta}^{(m)}$, and monitoring their convergence to one another. The computational details involved by implementing this procedure for computing ω_b are discussed in Sec. 2.2.4.

2.2.3 Outer Iteration Computational Considerations

The obvious ultimate goal of the outer iteration procedure is to be able to apply the Chebyshev acceleration procedure given in Eqs. (2.60) with accurate estimates of both λ_0 and $\bar{\sigma}$. However, since neither λ_0 and $\bar{\sigma}$ are known when the outer iterations are commenced, a "boot-strap" process is required. As reported in Refs. 12 and 13, it has been found advantageous to perform a limited number of power iterations, Eq. (2.50), initially to provide a reasonable estimate of λ_0 and an initial estimate of $\bar{\sigma}$, which is generally quite low. A series of low-order extrapolation cycles are then utilized, during which the higher overtones are rapidly damped out and more accurate estimates of $\bar{\sigma}$ are obtained. Only when all but the first overtone mode are essentially damped out are high-order cycles based on accurate estimates of $\bar{\sigma}$ utilized.

The precise algorithm can be described in terms of four basic parts as follows:[13]

1. A minimum of three power iterations using Eq. (2.50) are performed initially. The first Chebyshev acceleration cycle is begun on outer iteration n*+1, where n*+1 is the smallest integer such that n*>3 for which the dominance ratio estimate, $\hat{\sigma}$ satisfied the criterion

$$0.4 < \hat{\sigma} < 1.0,$$

where Eq. (2.68) is used to estimate $\bar{\sigma}$. That is,

$$\hat{\sigma} = E^{(n^*)}. \tag{2.83}$$

2. Using $\hat{\sigma}$ as the dominance ratio estimate for $\hat{\sigma}$ in Eq. (2.61), the accelerated iterative sequence given by Eq. (2.60) is carried out for iterations n*+p, p>1. At first, low degree polynomials are applied repeatedly, with the estimates of the dominance ratio being updated continuously according to

$$\hat{\sigma}' = \frac{\hat{\sigma}}{2}\left\{\cosh\left[\frac{\cosh^{-1}(\gamma)}{p-1}\right] + 1\right\}, \tag{2.84}$$

where

$$\gamma = C_{p-1}\left(\frac{2-\hat{\sigma}}{\hat{\sigma}}\right) E_{n^*,p-1}, \tag{2.85}$$

$$E_{n^*,p-1} = \frac{\| \underline{\psi}^{(n^*+p)} - \tilde{\underline{\psi}}^{(n^*+p-1)} \|_2}{\| \underline{\psi}^{(n^*+1)} - \tilde{\underline{\psi}}^{(n^*)} \|_2}, \tag{2.86}$$

and C_{p-1} is the Chebyshev polynomial of degree p-1. The polynomials are at least of degree 3 and are terminated when the error reduction factor $E_{n^*,p-1}$ is greater than the theoretical error reduction factor:

$$E_{n^*,p-1} > \left[C_{p-1}\left(\frac{2 - \hat{\sigma}}{\hat{\sigma}}\right)\right]^{-1}. \tag{2.87}$$

The theoretical error reduction factor is the error reduction which would have been achieved if $\hat{\sigma}$ were equal to $\bar{\sigma}$, the true dominance ratio. If $E_{n^*,p-1}$ is greater than this, the acceleration cycle has not been as effective as it should have been, so a new cycle is started using the updated dominance ratio estimate, $\hat{\sigma}'$, from Eq. (2.84).

It has been found judicious to limit the rate of growth of the dominance ratio estimates, $\hat{\sigma}'$, during the early stages of the iterative process. Denoting the dominance ratio estimate to be used to start a new polynomial cycle (p=1) at iteration n*+1 as $\hat{\sigma}$, $\hat{\sigma}$ is constrained as

$$\hat{\sigma} = \begin{cases} \min(\hat{\sigma}', 0.9) & , n^*+1 < 6 \\ \min(\hat{\sigma}', 0.95) & , n^*+1 < 9 \\ \min(\hat{\sigma}', 0.985) & , n^*+1 < 12 \\ \min(\hat{\sigma}', 0.99) & , n^*+1 > 12 \end{cases} \tag{2.88}$$

Though seldom needed in fast reactor problems, these constraints help smooth the convergence process in problems characterized by large dominance ratios.

3. After the estimates for $\bar{\sigma}$ have converged, higher degree polynomials are applied. In fact, the process described in part 2 above is applied continuously. The length of the cycles increases naturally due to the improving estimates of $\bar{\sigma}$.

4. The outer iterations are terminated at outer iteration n if the following three criteria are met:

$$\epsilon^{(n)} < \epsilon_\lambda, \tag{2.89}$$

$$\frac{\| \underline{\Psi}^{(n)} - \tilde{\underline{\Psi}}^{(n-1)} \|_2}{\langle \underline{\Psi}^{(n)}, \tilde{\underline{\Psi}}^{(n-1)} \rangle^{1/2}} < \epsilon_\psi , \tag{2.90}$$

$$\left| k_{eff}^{(n)} - k_{eff}^{(n-1)} \right| < \epsilon_k , \tag{2.91}$$

where ϵ_λ, ϵ_ψ and ϵ_k are input parameters. The test specified in Eq. (2.89) is a measure of the pointwise eigenvector convergence and is based on the bounds placed on the relative point error in the relationship (2.66). In computing $\varepsilon^{(n)}$, only cells in which the fission source has some minimum (user-specified) relative size are considered. The test (2.90) is a measure of the average rate of convergence of the eigenvector (the fission source), while test (2.91) is a measure of the eigenvalue convergence. The k_{eff} estimate at the end of n iterations is taken from

$$k_{eff}^{(n)} = k_{eff}^{(n-1)} \frac{\langle \underline{\psi}^{(n)}, \underline{\psi}^{(n)} \rangle^{1/2}}{\langle \underline{\psi}^{(n)}, \underline{\tilde{\psi}}^{(n-1)} \rangle^{1/2}} \tag{2.92}$$

Experience has shown that if ϵ_λ and ϵ_ψ are assigned equal values, the test (2.89) almost always controls convergence. The same tests (2.89)-(2.91) are applied after each outer iteration is completed, regardless of whether the iteration just completed was a power iteration or an accelerated iteration.

2.2.4 Inner Iteration Computational Considerations

Computational considerations arise concerning three aspects of the inner iterations. These are the computation of the optimum overrelaxation factor ω_b for each group, the determination of the number of inner iterations which should be carried out for a given group at a particular outer iteration and the actual procedure used to solve the tridiagonal matrix equations which characterize the line successive overrelaxation method.

It has been shown in Sec. 2.2.2 that the optimum overrelaxation factor for a given group can be computed if the spectral radius of the line Gauss-Seidel matrix, $\rho([L_1])$, is known. The procedure outlined in Eqs. (2.79)-(2.81) provides a rigorous method for determining $\rho([L_1])$. With the coding to carry out the inner iterations using the line successive overrelaxation method already in place, the implementation of this procedure is trivial, since $[L_1]$ is equal to $[L_\omega]$ with ω set to unity. The vector $\underline{k}_g$ in Eq. (2.75) also has to be set to the null factor.

In order to insure that the actual outer and inner iterations are as efficient as possible, this computation of the overrelaxation factors is done prior to commencing the first outer iteration. Starting with an arbitrary non-negative initial guess $\underline{x}^{(0)}$, the iteration in Eq. (2.79a) is carried out for m = 1 to 10. Following each iteration for m > 10, the quantities $\delta^{(m)}$, $\bar{\delta}^{(m)}$ and $\underline{\delta}^{(m)}$ are computed. The related quantities $\omega^{(m)}$, $\bar{\omega}^{(m)}$ and $\underline{\omega}^{(m)}$, defined by[12]

$$\omega^{(m)} \equiv \frac{2}{1 + (1 - \lambda^{(m)})^{1/2}} ,$$

$$\bar{\omega}^{(m)} \equiv \frac{2}{1 + (1 - \bar{\lambda}^{(m)})^{1/2}}, \tag{2.93}$$

and

$$\underline{\omega}^{(m)} \equiv \frac{2}{1 + (1 - \underline{\lambda}^{(m)})^{1/2}} ,$$

are also computed. The iterations for a given group are terminated when either

$$\left| \bar{\omega}^{(m)} - \underline{\omega}^{(m)} \right| < \frac{2 - \omega^{(m)}}{5} , \tag{2.94}$$

or $m = M$, where M is a user controlled iteration limit; ω_b for that group is set to $\omega^{(m)}$. The test given by Eq. (2.94) forces tighter convergence as $\rho([L_\omega])$ increases. The amount of CPU time required to precompute the ω_b is typically on the order of one or two outer iterations.

The theory presented in Sec. 2.2.1 on the Chebyshev acceleration method implicitly assumes that the matrix equation for each group, Eq. (2.72), is solved exactly during each outer iteration. For multidimensional problems, this is not the case. It has been shown[13] that the effect of solving Eq. (2.72) iteratively to less than infinite precision for each group is to modify somewhat the system of equations being solved. Although both systems share the same fundamental eigenvalue and eigenvector, the dominance ratio of the modified system is larger than the original system, Eq. (2.48). Some of the eigenvalues of the modified system may be negative or complex, which would slow convergence of the outer iterations.

The most practical solution to this problem is to do a sufficient number of inner iterations for each group during each outer iteration so that the effect on the dominance ratio is not appreciable, yet no more than this. It has been determined experimentally for a range of typical fast reactor problems[11] that this can be achieved most economically by doing a fixed number of iterations, m_g, for each group during each of the outer iterations. This eliminates the need for any convergence checking during the inner iterations and thus eliminates the costly divides which would have to be done to determine relative convergence on a component-by-component basis.

This number m_g is determined for each group by requiring that the norm of the continued product of the iteration matrices for that group during each outer iteration be less than some desired (user controllable) error reduction factor. This assures that the norm of any of the components of the error vector is greater than or equal to this error reduction factor during each

outer iteration. For a variant of the line successive overrelaxation method of Eq. (2.75), where a single Gauss-Seidel iteration precedes (m-1) successive overrelaxation iterations, the norm of the continued product of the iteration matrices is given by[26]

$$\left\| [L_{\omega_b}^{m-1}][L_1] \right\|_2 = [t_{2m-1}^2 + t_{2m}^2]^{1/2}, \quad m > 1, \tag{2.95}$$

where

$$t_m = [\omega_b - 1]^{(m-1)/2} \cdot [\rho(L_1)]^{1/2} [1 + (m-1)(1 - [\rho(L_1)]^{1/2})]. \tag{2.95b}$$

The single Gauss-Seidel iteration is applied because the norm in Eq. (2.95a) is then strictly decreasing for $m > 1$. Letting ε_{in} be the desired error reduction factor and given ε_b and $\rho(L_1)$ for a group from the optimum overrelaxation factor calculation just described, Eq. (2.96) is solved to determine that value of m such that

$$\left\| [L_{\omega_b}^{m-1}][L_1] \right\|_2 < \varepsilon_{in}. \tag{2.96}$$

The value of m so obtained is the fixed number of inner iterations, m_g, that are done for group g for every outer iteration. There is no direct user control over m_g; it is always computed from ε_{in}.

Experience has shown that choosing $\varepsilon_{in} \leq 0.04$ will result in no adverse impact on the outer iteration convergence rate for typical fast reactor problems. For problems with dominance ratios larger than 0.85 (large reactors), a value of ε_{in} as small as 0.01 is sometimes necessary. It is quite obvious when a value of ε_{in} which is too large for the problem at hand has been chosen. The dominance ratio estimates being obtained from the outer iteration grow too large, and oscillatory behavior of the acceleration cycles generally results.

A great percentage of the total CPU time required to solve large problems with this solution method is spent in the inner iterations. In implementing the algorithms used to carry out these iterations, it is essential that the full capabilities of the large-scale scalar scientific computers for which DIF3D was designed be utilized. A feature shared by some of these computers is the high speed instruction stack, from which significant gains in execution speed can be obtained when repetitive instruction sequences can be contained in this stack. Multiple functional units and instruction segmentation permit parallel execution of several arithmetic operations, loop indexing and the storing and fetching of data.

The requirements for utilizing these features efficiently include the following: (a) compact coding for loops, (b) no conditional branching performed within the loop, and (c) avoiding divisions whenever possible. The one-line successive overrelaxation method was chosen in part because it is simple and can be coded compactly. Performing a fixed number of inner iterations for each group eliminates the need for the divides and conditional branching which usually accompanies convergence checking. Finally, by utilizing

the procedure outlined below, it is possible to eliminate all divides and conditional branching from the innermost loops of the inner iteration algorithm and reduce those loops to a few lines of machine language coding which easily fit within the instruction stack on, say, an IBM 370/195 or a CDC 7600.

For a particular line of fluxes which are computed simultaneously during each inner iteration, the equations which must be solved are of the form

$$[A^x_{jk}]\hat{\underline{\phi}}^{(m+1)}_{jk} = \underline{s}_{jk}, \tag{2.97}$$

$$\underline{\phi}^{(m+1)}_{jk} = \omega_b(\hat{\underline{\phi}}^{(m+1)}_{jk} - \underline{\phi}^{(m)}_{jk}) + \underline{\phi}^{(m)}_{jk}, \tag{2.98}$$

$$\underline{s}_{jk} = q_{jk} + [A^y_{jk}]\underline{\phi}^{(m+1)}_{j-1k} + [A^y_{j+1k}]\underline{\phi}^{(m)}_{j+1k} + [A^z_{jk}]\underline{\phi}^{(m+1)}_{jk-1} + [A^z_{jk+1}]\underline{\phi}^{(m)}_{jk+1} \tag{2.99}$$

where j and k are the row and plane indices of this line, $[A^s_{jk}]$ are the matrices given by Eqs. (2.37)-(2.39) and the flux values ϕ_{0k} and ϕ_{J+1k}, k=1,2,...,K, and $\underline{\phi}_{j0}$ and $\underline{\phi}_{jK+1}$, j=1,2,...,J are null. The solution of Eq. (2.97) utilizes a variant of Gaussian elimination to perform the LU factorization of the tridiagonal matrix $[A^x_{jk}]$.

The forward elimination on the matrices $[A^x_{jk}]$ is performed only once, prior to the beginning of the outer iterations, in such a fashion as to eliminate the need for further divides in computing the $\underline{\phi}_{jk}$. The backward sweep and overrelaxation are then combined in a single loop to save memory fetches and stores.

We define $\ell_i \equiv a^x_i$ in Eq. (2.37) then the forward elimination on $[A^x_{jk}]$ is

$$d_1 = \frac{1}{b_1}, \tag{2.100a}$$

$$\left.\begin{aligned} u_i &= \ell_i d_{i-1} \qquad (2.100b)\\ d_i &= \frac{1}{b_i - \ell_i u_i} \qquad (2.100c)\end{aligned}\right\} \; i = 2, 3, \ldots, I.$$

The d_i values are saved for subsequent use in the inner iterations by storing over the b_i values, which are no longer needed. Given $\underline{s}_{jk}$ for one inner iteration, the forward sweep on it is given by

$$y_1 = s_1 d_1, \tag{2.101a}$$

$$y_i = (s_i + \ell_i y_{i-1})d_i, \quad i = 2,3, \ldots, I, \tag{2.101b}$$

where s_i is the i-th component of $\underline{s}_{jk}$. A second loop then performs the remainder of the work on line j,k according to

$$x_I = y_I, \quad \phi_I^{(m+1)} = \phi_I^{(m)} + \omega_b(x_I - \phi_I^{(m)}), \tag{2.102a}$$

$$\left.\begin{aligned} x_i &= y_i + \ell_{i+1} d_i x_{i+1} && (2.102b)\\ \phi_i^{(m+1)} &= \phi_i^{(m)} + \omega_b(x_i - \phi_i^{(m)}) && (2.102c) \end{aligned}\right\} \; i = I-1, \ldots, 2, 1.$$

This procedure permits very efficient use of the arithmetic capabilities of high speed scalar computers.

When periodic boundary conditions (e.g. next-adjacent-face periodicity or opposite-face periodicity) are present, the solution procedures given by Eqs. (2.97)-(2.102) require modification. The changes are minimized by permitting periodicity with respect to the domain boundary coincident with coordinate x_1, only. Consequently, next-adjacent-face periodicity couples the x_1 and y_1 faces; opposite-face periodicity couples the x_1 and x_I faces. The changes are summarized for two cases.

Case 1: Next-adjacent-face Periodicity

The following modifications are required:

(1) Replace diagonal element b_1 in $[A_{1k}^{gx}]$ (see Eq. (2.37) by

$$b_1^* = b_1 - a_1^x - a_1^y. \tag{2.103}$$

The elements of $[A_{jk}^{gx}]$ are unchanged for $j > 1$.

(2) Replace transverse leakage terms $s_i \equiv s_{ijk}$ in $\underline{s}_{jk}$ (Eq. (2.101)) by

$$s_{ijk}^* = s_{ijk} + \begin{cases} a_{i1k}^y \phi_{i1k}^{(m)} & j=1,\ i=2,3,\ldots,I \\ 0 & j=1,\ i=1 \\ a_{1jk}^x \phi_{j1k}^{(m+1)} & j>1,\ i=1. \end{cases} \tag{2.104}$$

Case 2: Opposite-Face Periodicity

The matrix $[A^{gx}_{jk}]$ associated with the opposite-face periodicity option has the special form (i.e. tridiagonal with two additional entries as indicated)

$$A^{gx}_{jk} = \begin{bmatrix} b_1 & -a^x_2 & & & & -a^x_1 \\ -a^x_2 & b_2 & -a^x_3 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & -a^x_{I-1} & b_{I-1} & -a^x_I \\ -a^x_1 & & & & -a^x_I & b_I \end{bmatrix}_{jkg} \tag{2.105}$$

where

$$a^x_1 \equiv a^{gx}_{1jk} = 2\left(\frac{\Delta x_1}{D_{1jk}} + \frac{\Delta x_I}{D_{Ijk}}\right)^{-1} A^x_{1jk} \tag{2.106}$$

The LU decomposition of this matrix is straightforward to derive. The resulting solution algorithm is summarized in the following equations.

Define $\ell_i \equiv a^x_i$, then the forward elimination sweep on $[A^{gx}_{jk}]$ and on $\underline{s}_{jk}$ is given by

$$\theta_0 = 1, \qquad \alpha_1 = 1, \qquad \Sigma_{\theta\alpha} = 0 \tag{2.107a,b,c^1}$$

$$u_1 = \ell_1, \qquad d_1 = b_1^{-1}, \qquad y_1 = s_1 d_1 \tag{2.107d,e^1,f^2}$$

$i = 2,3,\ldots I-1$

$$\theta_{i-1} = \theta_{i-2} u_{i-1} \tag{2.107g}$$

$$\alpha_i = \alpha_{i-1} \ell_{i-1} d_{i-1} \tag{2.107h}$$

$$\Sigma_{\theta\alpha} = \Sigma_{\theta\alpha} + \theta_{i-1}\alpha_i \tag{2.107i^1}$$

$$u_i = \ell_i d_{i-1} \tag{2.107j}$$

$$d_i = (b_i - \ell_i u_i)^{-1} \tag{2.107k^1}$$

$$y_i = (s_i + \ell_i y_{i-1}) d_i \tag{2.107ℓ^2}$$

$$\ell_I^* = \ell_I + \Theta_{I-2} u_{I-1} \tag{2.107m}$$

$$u_I = (\ell_I + \ell_{I-1} u_{I-1}) d_{I-1} \tag{2.107n}$$

$$d_I = (b_I - \ell_I^* u_I - \Sigma_{\theta\alpha})^{-1} \tag{2.107o[1]}$$

$$y_I = (s_I + \ell_I^* y_{I-1} + \sum_{i=1}^{I-2} \Theta_i y_i) d_I \tag{2.107p[2]}$$

Equations (2.107) may be arranged into two overlapping subsets so that the diagonal terms arising from the LU decomposition may be preinverted prior to the start of the outer iterations. Equations (2.107) with superscripts 1 or 2 apply to the preinversion step or the forward elimination of $\underline{s}_{jk}$, respectively. The non-superscripted Eqs. (2.107) apply to both steps.

The back substitution to complete the work on line j,k proceeds according to

$$\alpha_I = 0, \quad x_I = y_I, \quad \phi_I^{(m+1)} = \phi_I^{(m)} + \omega_b (x_I - \phi_I^{(m)}) \tag{2.108a}$$

$$\left.\begin{aligned} x_i &= y_i + \ell_{i+1} d_i x_{i+1} + \alpha_{i+1} x_I \qquad (2.108b) \\ \phi_i^{(m+1)} &= \phi_i^{(m)} + \omega_b (x_i - \phi_i^{(m)}) \qquad (2.108c) \end{aligned}\right\}, \quad i = I-1, \ldots, 2, 1.$$

The matrices $[A_{jk}^{gs}]$ obtained for triangular geometry options with non-periodic and periodic (next-adjacent-face periodicity only) boundary conditions are nearly identical to those obtained in the orthogonal geometry case. Consequently, the same general solution algorithms and data structures are applied.

Two aspects in which triangular geometry problems differ from orthogonal geometry problems lead to the two modifications detailed below.

First, because realistic reactor core models do not fully encompass either the rectangular or parallelogram problem domains required in the triangular geometry option, provision is made for the specification of background (unoccupied) mesh cells. Computational and physical considerations lead to the stipulation that the projection of the region of solution of the K planes be identical. Therefore, the majority of the background cells may be excluded from the calculation if iterations over line jk are over cells $i = I_j^s, I_j^s+1, \ldots, I_j^e$ where I_j^s and I_j^e are the first and last "active" mesh cells on a line. Occasionally, the reactor outer boundary is so irregular that one or more background mesh cells appear within the active mesh limits $I_j^s < i < I_j^e$ of a line. The leakage coefficients a_{ijk}^{gs} and the initial flux guess ϕ_{ijk}^{g} are set to zero in such a mesh cell, thereby permitting computations to proceed uninterrupted for the entire active mesh line.

The second difference between orthogonal and triangular geometry concerns the structure of the matrices $[A^{gy}_{jk}]$. Like their orthogonal geometry counterparts, the matrices $[A^{gy}_{jk}]$ have a single stripe. In the rectangular boundary domain option, this stripe is located on the main diagonal. In the parallelogram boundary domain option, however, the stripe is located either on the first super- or sub-diagonal of $[A^{gy}_{jk}]$ depending on the symmetry option (120° or 60°). In triangular geometry alternate elements of the diagonal stripe are zero corresponding to the fact that alternate y direction surface areas are nonexistent in the mesh ordering chosen here (see Figs. 2.4-2.6).

Thus in general the matrix $[A^{gy}_{jk}]$ is defined (for I odd, say) by

$$[A^{y}_{jk}] = \begin{bmatrix} a_1^{90} & a_2^{120} & & & & & & \\ a_2^{60} & 0 & 0 & & & & & \\ & 0 & a_3^{90} & a_4^{120} & & & & \\ & & a_4^{60} & 0 & 0 & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & a_{i-1}^{60} & 0 & 0 & \\ & & & & & 0 & a_I^{90} & \end{bmatrix}_{jk} \qquad (2.109)$$

where a^{t}_{i} denotes the coupling coefficient a^{y}_{ijk} corresponding to geometry option t. When option t is active all elements $a^{t'}_{i}$, $t' \neq t$ are zero. Note that t=90 denotes all rectangular domain symmetry options (e.g. 90°, 180° or 360°). When $t \neq 90$, the pattern of null super- or sub-diagonal elements is fixed. When t=90, the null entries begin on odd or even mesh cell indices depending upon the orientation of the first triangle in a given row. Knowledge of this special substructure of the $[A^{gy}_{jk}]$ leads to the following general algorithm for calculating the transverse leakage source in triangular geometry:

$$s_{ijk} = q_{ijk} + a^{z}_{ijk}\phi_{ijk-1} + a^{z}_{ijk+1}\phi_{ijk+1} + s^{y}_{ijk} \text{ for all } i,j,k \qquad (2.110)$$

where the same conditions apply to Eq. (2.110) as apply to the orthogonal geometry algorithm Eq. (2.99). The term s^{y}_{ijk} is defined by

$$s^{y}_{1,j,k} = a^{y}_{1+\ell,j+1,k}\phi_{1+\ell,j+1,k} \qquad j=1,2,\ldots,J-1, \quad i=1 \text{ and } t_j=2 \qquad (2.111a)$$

$$s^y_{i+1,j,k} = a^y_{i+1+\ell,j+1,k}\phi_{i+1+\ell,j+1,k} \qquad j=1,2,\ldots,J-1 \qquad (2.111b)$$

$$s^y_{i,j,k} = a^y_{i,j,k}\phi_{i-\ell,j-1,k} \qquad j=2,3,\ldots,J \qquad (2.111c)$$

$$\left.\begin{array}{l} i=t_j, t_j+2, \ldots, I^e_j - m_j \end{array}\right\}$$

$$s^y_{i,j,k} = a^y_{i,j,k}\phi_{i-\ell,j-1,k} \qquad j=2,3,\ldots,J,\ i=I^e_j,\ m_j=2 \qquad (2.111d)$$

$$s^y_{i,j,k} = 0 \qquad \text{otherwise} \qquad (2.111e)$$

where

$$t_j = \begin{cases} 1 & : \text{ parallelogram boundary domain (60° symmetry)} \\ 2 & : \text{ parallelogram boundary domain (120° symmetry)} \\ \text{mod}(j+\text{NTHPT},2)+1 & : \text{ rectangular boundary domain (NTHPT*=1 or 2)} \end{cases}$$

$$m_j = \text{mod}\,(I_j - t_j - 1,\ 2)$$

$$\ell = \begin{cases} 0 & : \text{ rectangular boundary domain} \\ -1 & : \text{ parallelogram boundary domain (60° symmetry)} \\ +1 & : \text{ parallelogram boundary domain (120° symmetry).} \end{cases}$$

2.2.5 Data Management Considerations

Strong consideration must be given to data management implications of any solution method that is contemplated for use in a code capable of treating problems where the number of space-energy unknowns can exceed 10^6. From the previous sections, it is obvious that such considerations have influenced the form of the solution method presented here. These considerations are summarized in this section.

The prime goal of the solution strategy described here is to reduce the number of outer iterations to a minimum, even at the expense of investing relatively greater effort in the inner iterations performed during each outer iteration. By minimizing the number of outer iterations, the number of scattering source calculations (one per group per outer iteration) is kept at a minimum. These scattering source calculations necessitate the transfer of large amounts of data from peripheral storage to core memory for problems utilizing 10 or more energy groups, yet there is little arithmetic to be done while these data transfers are taking place. As a result, CPU utilization can be quite low during the scattering source calculations, even if efficient asynchronous data transfer methods are utilized.

Data management considerations also led to the decision to apply the Chebyshev polynomial acceleration technique to the fission source vector $\underline{\psi}$ rather than the flux vector $\underline{\Phi}$. Three complete fission source or flux vectors,

*NTHPT denotes the orientation of the (1,1,1) triangle in the region of solution, see the GEODST file description in Appendix C.2.

depending on which are to be accelerated, have to be stored on peripheral storage devices and transferred to memory to carry out the acceleration procedure for each outer. Again, there is little arithmetic associated with this acceleration method, so that CPU utilization can again be low if large amounts of data have to be transferred. Since the fission source vectors are only (1/G) as long as the flux vectors, a significant reduction in data transfer requirements is achieved by accelerating the $\underline{\psi}$ vector.

Because fast reactor models are generally characterized by significantly fewer space mesh cells than thermal reactor models for reactors of the same thermal rating, relatively less effort is required to carry out the inner iterations for a given group in a typical fast reactor calculation. It is only for relatively large three-dimensional problems that all of the data required for the inner iterations for one group cannot be contained in the memory of the large scale computers available today. The spectral radii of the inner iteration matrices for the groups in a typical heterogeneous fast reactor problem are generally lower than those that arise from typical thermal reactor problems. Thus fewer iterations are required to achieve a given amount of error reduction in typical fast reactor problems. This lessens the price paid for demanding tighter convergence of the inner iterations in order to minimize the number of outer iterations.

Many relatively large three-dimensional problems that cannot be core contained may be solved with no appreciable increase in data transfer cost by employing the concurrent inner iteration strategy. Instead of calculating $\underline{\phi}_{jk}^{(m+1)}$ serially for all lines j,k, this strategy serially computes $\underline{\phi}_{jk}^{(m+1)}$ for the block of mesh planes currently core-contained, then computes all $\underline{\phi}_{jk}^{(m+2)}$,..., $\underline{\phi}_{jk}^{(m+B)}$ where B is the "active bandwidth" of core-contained mesh planes. If $B > m_g$, the number of inner iterations in group g, then the inner iterations require a single I/O pass comparable in cost to the one group core-contained option, but usually at a significantly reduced memory size requirement. Details of the concurrent inner iteration strategy are found in Section 4.3.2.2.

2.2.6 Adjoint Solution Strategy

The adjoint problem is solved using the same solution algorithm as the real problem. The self-adjoint property of the continuous and discretized within-group leakage-plus-removal operator only requires a transformation of data in order to utilize the iteration methods just discussed.

The transformation consists of:

(1) Reversing the order of the group structure of the principal macroscopic cross section data (e.g. $\Sigma_g^x \leftarrow \Sigma_{G+1-g}^x$).

(2) Transposing the scattering matrix (i.e. $T_{gg'} \leftarrow T_{g'g}$) and then reversing the order of the group structure (i.e. $T_{gg'} \leftarrow T_{G+1-g,G+1-g'}$). The corresponding arrays indicating the up and down (in)scatter bandwidth are converted to the corresponding up and down (out)scatter bandwidths.

(3) Interchanging $\nu\Sigma^{f}_{g'}$ and χ_g terms in the fission source calculation.

The resulting flux eigenvector is then obtained in reverse group order, g=G,G-1,...,1 and the fundamental eigenvalue is identical to the real problem due to the self-adjoint property of [Q] in Eq. (2.48). Likewise the symmetric within group matrices have identical spectral radii $\rho([L_{\omega_g}])$, hence the ω_g are identical.

2.2.7 Upscatter Iteration Strategy

DIF3D provides an upscatter iteration for application to problems in which $[T_{gg'}]>0$ for g'>g in Eq. (2.29). The essence of this strategy is to perform (in each outer iteration) U-1 additional group (inner) iterations for those groups within the upscatter bandwidth. Let $\bar{G}$ denote the group index of the first energy group that receives a nonzero upscattering source. Then the inner iterations for the groups without upscatter, g=1,2,...,$\bar{G}$-1, follow Eq. (2.72) and Eq. (2.73). The group g inner iteration at outer iteration n and upscatter iteration u is

$$[A_g]\underline{\phi}_g^{(n,u)} = \underline{b}_g^{(n,u)}, \qquad g = \bar{G}, \bar{G}+1, \ldots, G \tag{2.112a}$$

where

$$\underline{b}_g^{(n,u)} = \sum_{g'<g} [T_{gg'}]\underline{\phi}_g^{(n,u)} + \sum_{g'>g} [T_{gg'}]\underline{\phi}_g^{(n,u-1)} + \frac{1}{\lambda^{(n-1)}} \chi_g \underline{\Psi}^{(n-1)} \tag{2.112b}$$

$$\underline{\phi}_g^{(n,o)} = \underline{\phi}_g^{(n-1,U)} \tag{2.112c}$$

The calculation for the group contributions to the fission source $\underline{\psi}^{(n)}$ resume in the last upscatter iteration pass, U.

The cost of performing U upscatter iterations is approximately equivalent to solving a problem with (U-1)*(G-$\bar{G}$+1) additional groups. If a scattering band B of fluxes is core contained and if (G-$\bar{G}$+1)<B, then the upscatter iterations requires no additional I/O transfers for the flux data. Finite difference coefficients and cross section data transfers will still be required.

Experience with several Safety Test Facility configurations with thermal and epithermal drivers indicates that user-supplied U values between 5 and 10 are comparable in performance for the thermal case. U=1 is sufficient for the epithermal case.

The procedure in Eqs. (2.112) is reversed for adjoint calculations with upscatter. The upscatter iterations are performed in groups g=G,G-1,...$\bar{G}$. Then the remaining groups, g=$\bar{G}$-1,G-2,...,1 are calculated.

2.2.8 The Inhomogeneous Problem

The matrix equations describing the fixed distributed source problem may be written in the form

$$([M] - \mu[B])\underline{\phi} = \underline{S} \tag{2.113}$$

where [M] and [B] are defined by Eqs. (2.35) and (2.42), and $\underline{S}$ is the external source vector. The constant μ is specified to ensure the subcriticality of the reactor in the absence of an external source. An exception occurs, for example, in generalized perturbation theory adjoint calculations where the reactor is critical, but the adjoint source $\underline{S}$ is orthogonal to the fundamental mode; in this case a solution is guaranteed by the alternative theorem.[31] For this discussion μ=1 suffices, since [B] may be redefined. The flux $\underline{\phi}$ is subject to the boundary and interface conditions of Eqs. (2.3)-(2.5).

Equation (2.113) may be written as

$$\underline{\phi} = ([I] - [M]^{-1}[B])^{-1}\underline{u} \tag{2.114}$$

where $\underline{u} = [M]^{-1}\underline{S}$. The properties of [M] and [B] discussed in Section 2.2.1 together with the assumption of reactor subcriticality requires $\rho([M]^{-1}[B])<1$. Therefore, $([I]-[M]^{-1}[B])^{-1}$ exists which in turn implies that $([M]-[B])^{-1} = ([I]-[M]^{-1}[B])^{-1}$ exists. Because [M] is nonsingular, the iterative process

$$[M]\underline{\phi}^{n} = [B]\underline{\phi}^{n-1} + \underline{S} \tag{2.115}$$

for the flux $\underline{\phi}$ generated from the regular splitting[18,32] of ([M]-[B]) will converge.

The flux iteration is reduced to a fission source iteration by following the procedure outlined for the eigenvalue problem, provided the definition of $\underline{\phi}_g$ is appropriately modified for the fixed source problem, i.e.

$$\underline{\phi}_g = [L_g]\underline{\psi} + [A_g]^{-1}\left(\sum_{g'\neq g}[T_{gg'}]\underline{S}_{g'} + \underline{S}_g\right). \tag{2.116}$$

Then multiplying Eq. (2.113) by $[F]^T$ and using Eqs. (2.42) and (2.44) we obtain the reduced problem

$$\underline{\psi} = ([I]-[Q])^{-1}\underline{v}, \tag{2.117}$$

where $\underline{v} = [F]^T\underline{u}$ and [Q] is defined by Eq. (2.49). Because the nonzero eigenvalues of [Q] and $[M]^{-1}[B]$ are identical, $\rho([Q])<1$ and therefore $([I]-[Q])^{-1}$ exists. Consequently, the iterative process

$$\underline{\psi}^{n} = [Q]\underline{\psi}^{n-1} + \underline{v} \tag{2.118}$$

generated from a regular splitting of ([I]-[Q]) will converge and the fission source vectors obtained from the flux problem and the fission source problem will be identical.

The rate of convergence in fixed source problems is dependent on $\rho([Q])$. The Chebyshev acceleration method detailed in Section 2.2.1 can therefore be applied to the iterations in Eq. (2.118) provided that suitable estimates of $\rho(Q)$ are obtained. One such estimate may be obtained using Eq. (2.68), which for the fixed source problem is easily shown to satisfy the relation

$$\lim_{n\to\infty} E^{(n)} = \rho([Q]). \tag{2.119}$$

The previously described Chebyshev acceleration procedures may be used directly in fixed source problems, provided we redefine the meaning of the symbol $\bar{\sigma}$ to mean $\rho([Q])$, the spectral radius of the iteration matrix.

The inner iteration process in fixed source problems differs from its counterpart in eigenvalue problems only by the presence of an additional source term contribution to q_{jk} in Eq. (2.99).

When the fixed source problem is near-critical (i.e. $\rho([Q])$ approaches unity), convergence rates, even with Chebyshev acceleration are unacceptably slow. Application of a single asymptotic extrapolation[33,34] prior to the first Chebyshev acceleration significantly reduces the required number of iterations. This reduction is achieved by an approximation procedure that attempts to correctly scale the contribution of the fundamental eigenvector to the flux solution. This approach is motivated by the fact that in near-critical source problems the fundamental eigenvector term dominates the solution.

If we assume, therefore, that the n-th iterate of Eq. (2.118) converges to the exact solution $\underline{\psi}^{\infty}$ with asymptotic behavior

$$\underline{\psi}^{\infty} = \underline{\psi}^{(n)} + \rho^{n}([Q])c\underline{\psi}_{0}. \tag{2.120}$$

where $c\underline{\psi}_0$ is an arbitrary multiple of the fundamental eigenvector of [Q] corresponding to $\rho([Q])$, then it follows that an improved n-th iterate is

$$\tilde{\underline{\psi}}^{(n)} = \underline{\psi}^{(n)} + \tau^{(n)}(\underline{\psi}^{(n)} - \underline{\psi}^{(n-1)}) \tag{2.121}$$

where the extrapolation factor $\tau^{(n)}$ is defined by

$$\tau^{(n)} = \frac{\rho^{(n)}}{1-\rho^{(n)}}. \qquad (2.122)$$

Here, $\rho^{(n)} = E^{(n)}$ is the estimate for $\rho([Q])$ at the n-th unaccelerated power iteration.

As alluded to earlier, the effect of the extrapolation is to rescale the contribution of the fundamental vector to the solution. The extrapolation factor also increases[34] the magnitude of the higher harmonics. However, these are readily attenuated by the Chebyshev acceleration procedures that (after a single unaccelerated outer iteration) are applied to subsequent iterations.

To ensure that an asymptotic behavior has been achieved, the single extrapolation is performed when the following conditions are met:

1. $\varepsilon_\rho^{(n)} < .1$ (2.123a)

2. $\varepsilon_\rho^{(n-1)} < .1$ (2.123b)

3. $n \geq 5$ (2.123c)

where

$$\varepsilon_\tau^{(n)} = \frac{\tau^{(n)} - \tau^{(n-1)}}{\tau^{(n)}}. \qquad (2.123d)$$

The asymptotic extrapolation procedure typically leads to a factor of 2 or more reduction in the number of outer iterations required to achieve comparable fission source accuracy with the standard acceleration method.

2.3 The Criticality Search Option

2.3.1 Statement of the Problem

The criticality search[17] seeks to achieve a desired reactor k-effective, k_d, by adjusting certain parametric vectors which are constrained to lie along a given straight line. The parametric vectors considered here are subzone volume fractions which are discussed later in section 2.3.3. Other commonly used parametric vectors (not implemented in DIF3D) include buckling, dimension and reactor period (α).

If $\underline{p} = (p_1, p_2, \ldots, p_R)$ denotes a parametric vector, then the desired vector is constrained to lie on the line given by

$$\underline{p}(s) = \underline{p}_o + s \cdot \underline{\delta p} \qquad (2.124)$$

where $\underline{\delta p} = (\delta p_1, \delta p_2, \ldots, \delta p_R)$ denotes the parametric modifiers (the direction cosines for the line), and $\underline{p}_o$ denotes the initialized state of the parameter vector when s=0.

For reasonable* values of s and $\underline{\delta p}$, the parametric vector $\underline{p}(s)$ generates matrices [M(s)] and [B(s)] having the same general properties as the matrices [M] and [B] in Eq. (2.34). Then associated with each vector $\underline{p}(s)$ is $k_{eff}=k(s)$, the solution to the eigenvalue problem

$$[M(s)]\underline{\phi} = \frac{1}{k(s)} [B(s)]\underline{\phi} . \tag{2.125}$$

The object of any search then is to solve the equation

$$k(s) = k_d. \tag{2.126}$$

2.3.2 Method of Solution

The solution of Eq. (2.126) is achieved by repeatedly solving Eq. (2.125) for a series of carefully selected estimates s_n. This iterative process has three principle steps. The first step estimates s_n; Step 2 solves Eq. (2.125) for $k(s_n)$ and Step 3 performs the convergence check on $k(s_n)$.

Step 1: Estimation of s_n

s_1 and s_2 are derived from user data. s_3 is determined by linear interpolation or extrapolation of data from search passes 1 and 2:

$$s_n = s_{n-1} + e_{n-1}/(dk/ds)_{n-1} \tag{2.127}$$

where

$$e_n = k_d - k(s_n) \tag{2.128}$$

$$(dk/ds)_n = (k(s_n) - k(s_{n-1}))/(s_n - s_{n-1}). \tag{2.129}$$

When n>3, the three most recent estimates $\{s_{n-1}, s_{n-2}, s_{n-3}\}$ determine a parabola $p(s_i) = p_1 s_i^2 + p_2 s_i + p_3 - k(s_i)$, i = n-1,n-2,n-3. Then, s_n is the root of $p(s)-k_d=0$ that is closest to s_{n-1}.

*The user is expected to specify an initial configuration [M(0)] and [B(0)] that is reasonably close to the desired solution, and is expected to specify search parameter constraints that avoid non-physical configurations.

If the parabola is degenerate (a straight line) or if the roots of $p(s)-k_d=0$ are complex, then linear extrapolation is applied. The estimate having the largest e_i and which upon removal leaves two estimates that bracket the solution k_d will then be discarded (This is the regula falsi algoritm[35]).

If the parabola is not degenerate, a similar root bracketing procedure is used to discard in favor of s_n the least useful estimate among s_{n-1}, s_{n-2} and s_{n-3}.

Step 2: Solution of Eq. (2.125)

The eigenvalue problem Eq. (2.125) is solved using the methods discussed for Eq. (2.43). The matrices [M(s)] and [B(s)] are defined by

$$[M(s)] = [M(0)] + \lambda[\delta M] \tag{2.130a}$$

$$[B(s)] = [B(0)] + \lambda[\delta B] \tag{2.130b}$$

where [M(0)] and [B(0)] denote the matrices obtained with no contributions from the search ("modifier") subzones and $\lambda[\delta M]$ and $\lambda[\delta B]$ denote the matrix of perturbations resulting from the inclusion of the search modifier subzones. $[\delta M]$ and $[\delta B]$ have the same general structure as [M] and [B], but the former are quite sparse due to the limited number of compositions usually modified during a search.

Step 3: Termination Tests

Search passes are terminated by any one of the following events:

1. $k_d - k(s_n) < \varepsilon_d$ where ε_d is a user-supplied threshold;

2. $n = n_{max}$ where n_{max} is a user-supplied iteration limit;

3. $s_n < s_{min}$ and $s_n > s_{max}$ where s_{min} and s_{max} are minimum and maximum limits on the range of s. The first time s_n exceeds the search range say, $s_n < s_{min}$, it is set to s_{min}. A subsequent violation of the limits cause termination.

4. Insufficient time remains to perform the next eigenvalue calculation.

2.3.3 Comments on the Concentration Search Option

On each search pass the SRCH4C module rewrites the subzone[6] volume fractions on the CCCC file NDXSRF and the HMG4C module calculates the corresponding macroscopic cross sections for the code-dependent file COMPXS. This approach is attractive for two reasons. First, the creation of "modifier" subzones (i.e. collections of isotopes or materials which are to be varied during the search) requires minimal effort on the part of the user. During the search

process it is a trivial matter for SRCH4C to rewrite the subzone volume fractions on the NDXSRF file. The second advantage of this approach is modularity. Arbitrary neutronics computation modules that use the CCCC interface files may be employed to solve the eigenvalue problem.

The alternative to subzone volume fraction modification requires atom density modification for all nuclides in the CCCC file ZNATDN, a job of considerably larger magnitude that yields a marginal improvement in user convenience.

The economics of incurring the overhead associated with repeated exits and reentries to the neutronics module might argue against the modular approach. The net gain from avoiding such overhead was considered marginal compared to the benefits of modularity.

Except for the prompt fission spectrum cross section type, the modification of subzone volume fractions in "modifier" subzones yields the following homogenization equation

$$\Sigma_m^{x,g} = \sum_{i\epsilon m_o} \sigma_i^{x,g} n_{im_o} V_{im_o}^f + s_n \sum_{i\epsilon m_s} \sigma_i^{x,g} n_{im_s} \qquad (2.131)$$

where

$\Sigma_m^{x,g}$ is the macroscopic cross section of type x for group g in zone m;

$\sigma_i^{x,g}$ is the microscopic cross section of type x for group g for isotope i;

m_o denotes the set of isotopes in the primary zone assignment and subzone assignments of zone m (modifier subzones are excluded);

m_s denotes the set of isotopes in modifier subzone assignments of zone m;

n_{im} is the atom density of isotope i in the appropriate set m_o or m_s;

V_{im}^f is the zone or subzone volume fraction assigned to isotope i in the set $m = m_o$ or m_s.

Equation (2.131) may be viewed from a macroscopic standpoint as

$$\Sigma_m^{x,g} = \Sigma_{m_o}^{x,g} + s_n \delta\Sigma_{m_s}^{x,g} \qquad (2.132)$$

where

$$\Sigma_{m_o}^{x,g} = \sum_{i\epsilon m_o} \sigma_i^{x,g} n_{im_o} V_{im_o}^f \qquad (2.133a)$$

and

$$\delta\Sigma^{x,g}_{m_s} = \sum_{i\epsilon m_s} \sigma^{x,g}_i n_{im_s} . \qquad (2.133b)$$

Modification of the prompt fission spectrum cross section depends upon which of the three available homogenization options are selected.

Option 1: Use set χ vector for all zones

$$(\chi^g_m)_n \equiv (\chi^g). \qquad (2.134)$$

Option 2: Use isotope fission vectors with total fission source weighting

$$(\chi^g_m)_n = \frac{\sum_{i\epsilon m} (\chi^g_i)_{n_{im}} V^f_{im} \sum_{g'} (\nu\sigma_f)^{g'}_i}{\sum_{i\epsilon m} n_{im} V^f_{im} (\nu\sigma_f)^g_i} \qquad (2.135)$$

where $V^f_{im} = s_n$ for those isotopes in search modifier subzones.

Option 3: Use isotope fission vectors with $(\nu\sigma_f)$ weighting

$$(\chi^g_m)_n = \frac{\sum_{i\epsilon m} (\chi^g_i)_{n_{im}} V^f_{im} (\nu\sigma_f)^g_i}{\sum_{i\epsilon m} n_{im} V^f_{im} (\nu\sigma_f)^g_i} . \qquad (2.136)$$

There are no restrictions on subzone modifiers or on the zone being modified with regard to fissionable or nonfissionable cross section types or with regard to scattering bandwidths.

2.4 Summary

The mesh-centered finite-difference approximation introduces a three-, five- or seven-stripe symmetric matrix of coupling coefficients that are computed using Eqs. (2.25)-(2.27); Tables 2.1 and 2.2 summarize formulas associated with each geometry option. The required source term is computed using Eq. (2.28) and Eq. (2.2). During each inner iteration a particular line of fluxes is simultaneously computed by solving Eqs. (2.97)-(2.99).

For a wide class of LMFBR problems no user input is required by the acceleration strategies described in Sections 2.2.1-2.2.4. On option the user may override ϵ_{in}, the inner iteration error reduction factor in Eq. (2.96), which influences the fixed number of inner iterations to be performed during the within-group calculations in each outer iteration. Section 3.15.2 addresses performance issues in this regard. Performance (i.e. job cost) is also directly related on many host installations to the user-specified ECM storage container size, ultimately the job memory size. Sections 3.9.1 and 3.10.1 address this issue.

3. A GUIDE FOR USER APPLICATIONS

3.1 Setting Up a DIF3D Job - An Overview

As mentioned in the introduction, the code described in this report is, in fact, a collection of quite independent code blocks. DIF3D actually is only one of these code blocks; the others process input data required by the diffusion-theory calculation. It is a common, though sometimes confusing, practice to apply the name "DIF3D" to both the complete set of code blocks and the specific diffusion-theory calculation code block.

The DIF3D code block itself reads only binary files. Other code blocks read card input and convert the data to binary files. The input to the code, therefore, is generally a mix of binary files written by code blocks and card-image files composed by users. Users have a variety of options available in choosing the mix; their choice then determines which code blocks are actually executed.

This section is a brief overview of the input requirements. Later sections go into greater detail. Information regarding specific input data sets or conventions may be rapidly located by using the table of contents with its detailed subsection headings.

3.1.1 Input Binary Files

In practice the input to DIF3D (the collection of code blocks) usually includes only a few binary files. Unless otherwise noted these files will be one of the CCCC interface files described in Appendices C.1 - C.10.

Microscopic cross section libraries are usually maintained as binary files; DIF3D can use two alternative formats, ISOTXS or the code-dependent file XS.ISO (see Ref. 36).

For restart and in cases where reasonable flux guesses are available the binary flux file RTFLUX may be input. The adjoint flux is stored in the binary file ATFLUX.

Other input binary files may contain macroscopic cross sections (COMPXS) (see Appendix D.1), atom number densities (NDXSRF,ZNATDN), geometry specifications (GEODST), inhomogeneous sources (FIXSRC), criticality search parameters (SEARCH) and code-dependent data (DIF3D) (see Appendix D.2). Files in this group are rarely input to the code; it is usually simpler to supply data in card-image form.

3.1.2 BCD Card-Image Model Input

When input data are not provided in binary files one or more of the input processors will be evoked to read BCD card-image files and to write appropriate binary files. This is done automatically; users do not have to provide any special instructions.

BCD input is divided into a number of blocks of data called "DATASETs". The general BCD input format for DIF3D is described in a later section of this chapter; the card-by-card input descriptions are included in the Appendices B.1-B.4.

Atom number densities, geometry specifications, inhomogeneous sources and criticality search parameters can all be input in the A.NIP3 DATASET (see Appendix B.4).

Microscopic cross sections can be input in BCD form in A.ISO (see Appendix B.3), a BCD equivalent of ISOTXS.

Finally, at Argonne any of the CCCC files[6] ISOTXS, RTFLUX, ATFLUX, NDXSRF,ZNATDN, GEODST, FIXSRC, and SEARCH can be generated directly from the DATASET A.LASIP by the LASIP3 code[37]. LASIP3 is a Los Alamos National Laboratory input processor.

3.1.3 BCD Card-Image Calculation Parameter Input

Two DATASETs, A.DIF3D and A.HMG4C, contain input parameters for the diffusion-theory calculation and the cross section homogenization, respectively. In practice these DATASETs usually contain only a few cards. Nearly all the parameters have defaults which have been set within the coding to values appropriate for a wide range of problems.

Among the more important input job parameters are the sizes of the FCM (fast core) and ECM (extended core) data containers. In several places (e.g. A.NIP3, A.DIF3D, A.HMG4C) the user may override defaults and specify the amount of core individual code blocks are to use for data storage. Even on machines with only one level of memory (e.g. IBM machines) two containers are required.

3.1.4 Edits

Individual code blocks offer a variety of edits, most of which can be controlled by the user via input flags. Because most code blocks are independent programs it frequently happens that particular data can be edited from several different places in the code. For example, macroscopic cross sections can be edited in the code block that performs the homogenization (HMG4C) or in the diffusion-theory solution (DIF3D).

Most edits can be routed to one or both of two output media by means of the edit flags. The regular print file (logical unit 6 at Argonne) is normally a printer; the auxiliary print file (logical unit 10 at Argonne) may be any device the user chooses (e.g. microfiche or a disk file).

3.2 BCD Input Conventions

In the input convention used in DIF3D and most other Applied Physics codes, the input BCD card images are grouped into "BLOCKs", and the card images within each BLOCK are grouped into "DATASETs". BLOCKs and DATASETs are identified by cards containing one of the following phrases:

```
BLOCK=blknam
DATASET=dsname
UNFORM=dsname
NOSORT=dsname
MODIFY=dsname
REMOVE=dsname
```

The words to the left of the "=" sign are "keywords"; the words to the right of the "=" sign are unique BLOCK or DATASET names. Keywords must start in column 1 of the card, and there can be no imbedded blanks.

Both binary and BCD files are given names and, following the CCCC conventions,[6] version numbers. Binary files include CCCC standard interface files, code dependent interface files for passing data between load modules, and scratch files used only within particular load modules. BCD files for Applied Physics codes are usually given names starting with "A."; for example A.NIP3 is the BCD file which defines the neutronics input geometry and isotopic number density data.

The number of versions permitted for a particular file is established by individual programs. In references in the BCD card input to one of several versions of a file, the version number must follow the file name and be separated from it by a comma. Taking examples from the list of keyword phrases above:

```
DATASET=A.SAMPLE,2
REMOVE=RTFLUX,1
```

A version number of unity is implied when no version number is given. Thus, the second example above could have been written:

```
REMOVE=RTFLUX
```

DIF3D users can normally ignore version numbers; the commonly used files come in only one version. The exceptions are the UDOIT binary files, which are intended for individual applications of DIF3D.

3.2.1 BLOCK=

The BCD input stream is divided into BLOCKs, and each BLOCK starts with a card containing

```
BLOCK=blknam
```

In the DIF3D input "blknam" may be either the word "OLD" or the word "STP021". The special case of BLOCK=OLD is discussed in a later section. STP021, which stands for "Standard Path 21", is the name given at Argonne to the sequence of modules making up a DIF3D calculation. A BLOCK ends at the last card before the next BLOCK= card or at the end of the card input file, whichever is encountered first.

As far as the user is concerned, the phrase BLOCK=STP021 causes the execution of a DIF3D job. If the phrase occurs twice in the input stream DIF3D is executed twice. Only data contained in the first BLOCK are available to the program during the first execution. Data in the second BLOCK modify or replace the first BLOCK data for the second execution.

3.2.2 DATASET=, UNFORM=, NOSORT=

The data within each BLOCK are subdivided into DATASETs, and each DATASET starts with a card containing one of the phrases:

```
DATASET=dsname
UNFORM=dsname
NOSORT=dsname
```

A DATASET ends at the last card before the next keyword or at the end of the card input file, whichever comes first. The order of dissimilarly named DATASETs within a single BLOCK makes no difference to the execution of the program.

DATASETs designated DATASET= or UNFORM= are expected to contain cards on which the first two columns contain either

1. a positive, 2-digit, nonzero "card type number," or

2. blanks, zeros or non-numeric characters.

The type numbers (01, 02, ... 99) are used to identify the type of data on each card. For example, in the BCD input file named A.NIP3 mesh data are supplied on "type 09 cards" (card-images that have "09" punched in columns 1-2).

At the beginning of each job the cards with card type numbers are automatically rearranged in order of ascending card type number in DATASETs specified by DATASET= or UNFORM=. When more than one card of a particular card type is present the relative order of those similarly numbered cards is unchanged.

At the same time as numbered cards are reordered, unnumbered cards (those with blanks, zeros or non-numeric characters in cols. 1-2) are collected and placed after all numbered cards. Some users use unnumbered cards as "comment cards" to annotate their decks of numbered cards; before the data are read by applications load modules the unnumbered comment cards are swept to the back of the DATASET where they will not be seen by the load module. A listing of the input deck before sorting is printed on the user's output medium so that the comments are available for documentation.

DATASETs designated NOSORT= are not reordered in any way. NOSORT DATASETs are normally used for data required by a load module which was written at another installation but which was incorporated as a load module in an Applied Physics production code. In DIF3D A.ISO and A.LASIP are NOSORT DATASETs.

Most DIF3D DATASETs can be input in either formatted or unformatted form. When prefaced by DATASET= the data must all be input in the formats specified in the input description for each card type. When prefaced by UNFORM= the data may be in free-format, but subject to the rules outlined later in this chapter in the section on free-format syntax. In either case cols. 1-2 are still reserved for card type numbers. The format rules for NOSORT DATASETs depend on the individual load modules which read them.

When BLOCK=blknam appears twice in the input - specifying two executions of the same sequence of load modules - DATASETS in the first BLOCK are automatically preserved for the second execution unless the user deliberately redefines a DATASET in the second BLOCK. For example,

```
BLOCK=STP021
DATASET=A.NIP3
01    data  ...
02    .........
07    .........
      .........
      .........
BLOCK=STP021
DATASET=A.NIP3
01    new data
02    .........
06    .........
```

The first DATASET is entirely replaced by the second before the second execution. A later section discusses how one can make selective changes to DATASETs.

3.2.3 BLOCK=OLD

The special BLOCK "OLD" permits the user to tell DIF3D which files already exist on disk and are being input to the calculation. Input disk files must be listed under BLOCK=OLD in the following manner:

```
BLOCK=OLD
DATASET=dsname
DATASET=dsname
    etc.
```

BLOCK=OLD may be placed anywhere in the BCD card input file.

These BLOCK=OLD files are usually binary library or restart files. Occasionally it may be convenient to create and save a BCD file in one job and then pass it to a second job on disk rather than in the BCD card input file. In such a situation the DATASET name should appear under BLOCK=OLD in the second job and not in any other BLOCK processed by the second job.

3.2.4 MODIFY=, REMOVE=, nn=DELETE

MODIFY=dsname permits the user to replace cards of a particular card type in an old DATASET without affecting the rest of the data. Type-numbered cards following MODIFY=dsname replace the cards of that type (or those types) in a previously defined DATASET. For example, if a DATASET in one BLOCK contains seven type 09 cards and five new type 09 cards are provided in a second BLOCK under MODIFY=dsname, then the seven original cards are deleted and the five new cards substituted before the second execution.

Some users like to define a reference DATASET with DATASET=dsname and then make changes in the same BLOCK before execution with MODIFY=dsname.

REMOVE=dsname deletes the entire DATASET. This option frequently is used with binary files to force applications load modules, for one reason or another, to rewrite a file.

nn=DELETE, where nn is a card type number, after a MODIFY=dsname will cause all of the type nn cards to be deleted from the DATASET.

3.2.5 Sample Input

Figure 3.1 shows a BCD card input file for a fictitious program. The input is designed to exercise most of the options described above. Three input DATASETs are defined; they are two separate versions of a file named A.SAMPLE and one named A.XAMPLE. Below the listing of the input, Figure 3.1 shows the contents of each file after preprocessing and before the imaginary program is executed. There are two BLOCKs (i.e. two executions in the job).

MODIFY= is used in the first BLOCK to modify a DATASET defined in the same BLOCK (A.SAMPLE,2). It is used in the second BLOCK to modify a DATASET defined in the first BLOCK (A.SAMPLE,1).

Note that A.SAMPLE,1 and A.SAMPLE,2 are defined with DATASET= and UNFORM=; the cards are reordered according to card type with unnumbered cards placed last. A.XAMPLE is defined with NOSORT= and is unaffected by the preprocessing.

3.2.6 Output from BCD Input Card Preprocessors

The BCD input preprocessing routines normally produce two kinds of edits. At the beginning of the job the user's input is listed on both the regular and auxiliary output print files by the routine SCAN. In addition, all DATASETs processed under each BLOCK=blknam are edited by the routine STUFF. Users have control over the STUFF edits for each BLOCK through an integer sentinel, n, that can be added to the BLOCK= card:

BLOCK=blknam,n

n = 0, edits given on both regular and auxiliary output files (default).
= 1, edits on regular output file only.
= 2, edits on auxiliary output file only.
= 3, no edits for the current BLOCK.

3.3 General Philosophy on Input Data

A number of principles have guided the design of BCD card input for DIF3D and other Applied Physics codes.

1. Data that are not essential to the problem should not be required in the BCD card input. In particular, no redundant data should be required.

2. Card input files should be easy to create and to modify.

3. Whenever possible, labels and names should be used instead of numbers for descriptive data.

The BCD input conventions defined in the previous section support these principles.

The convention of numbered cards containing very specific types of data helps to eliminate nonessential and redundant data. The preprocessing routines pass to the applications programs the number of cards of each type contained

```
BLOCK=TEST
DATASET=A.SAMPLE
    A.SAMPLE,1
09  09 CARD
05  1ST 05 CARD
 5  2ND 05 CARD
    UNNUMBERED
07  07 CARD
5   3RD 05 CARD
UNFORM=A.SAMPLE,2
XX  A.SAMPLE
XX  VERSION 2
08  08 CARD
MODIFY=A.SAMPLE,2
08  REPLACE 08
BLOCK=TEST
MODIFY=A.SAMPLE,1
09=DELETE
05  REPLACE 05
REMOVE=A.SAMPLE,2
NOSORT=A.XAMPLE
    A.XAMPLE
    NOSORT
07  TYPE 07 CARD
    NO NUMBER
07  ANOTHER 07
```

To the left is a sample input file illustrating many of the input processing options. There are two BLOCKs and three DATASETs referenced.

Contents of each of the three DATASETs after the first BLOCK is processed.

A.SAMPLE version 1	A.SAMPLE version 2	A.XAMPLE
05 1ST 05 CARD	08 REPLACE 08	not defined in
5 2ND 05 CARD	XX A.SAMPLE	the first BLOCK
5 3RD 05 CARD	XX VERSION 2	
07 07 CARD		
09 09 CARD		
A.SAMPLE,1		
UNNUMBERED		

Contents of each of the three DATASETs after the second BLOCK is processed.

05 REPLACE 05	not defined in	A.XAMPLE
07 07 CARD	the second BLOCK	NOSORT
A.SAMPLE,1		07 TYPE 07 CARD
UNNUMBERED		NO NUMBER
		07 ANOTHER 07

Fig. 3.1. Illustration of Input Conventions

in a particular DATASET. The user never has to tell a code how many data of a particular type are input; the code determines this fact independently. Default values can be provided not only when a particular datum is missing, but also when whole card types are missing.

About forty different card types are defined for the geometry and isotope number density file A.NIP3. Rarely are more than a dozen used for a particular job. Instead of user supplied sentinels, the presence or absence of particular card types signals options. Explicit sentinels would be redundant.

Numbered cards and the free-format option make it relatively easy to create and modify DATASETs. Long strings of input data and tables are convenient to the programmer but not to the user. Applied Physics input has always tended towards requiring only a few pieces of data per card, with the format of the card designed for the convenience of the user. In some cases cards of a particular type may be shuffled without affecting the definition of a problem. In other cases the order of cards within a card type has significance; the data on one card may overlay, in some way, data defined on a previous card. Modifications to input can frequently be made simply by adding or changing the order of cards; no changes to existing cards are required.

If nothing else, the use of labels instead of numbers for input quantities makes the BCD card input file readable to users. In the A.NIP3 DATASET, for example, compositions and geometric regions are given labels, and isotopes are referred to by name.

3.4 Free-Format (FFORM) Syntax Rules

Free-format input is processed by a subroutine named FFORM. The following set of rules applies to data prepared for UNFORM= DATASETs.

3.4.1 Delimiters

Data (integers, floating point numbers and Hollerith words) must be separated either by blanks or by combinations of one or more of the four special delimiters:

,	comma
(	left parenthesis
)	right parenthesis
/	slash

3.4.2 Data Forms

Integer and real numbers must be written according to the usual FORTRAN rules and may not have imbedded blanks. Hollerith data can be supplied in any of the following three ways:

1. A string of letters and numbers, beginning with a letter, with no imbedded blanks.

   e.g. U238 PU239

2. A string of symbols surrounded by asterisks or apostrophes. In the current version of FFORM for CDC machines only the asterisk can be used to set off Hollerith data; the apostrophe has not been implemented.

   e.g. *NA 23* 'REG1'

3. A string preceded by the Hollerith prefix nH, where n is an integer constant.

   e.g. 3H016

On IBM machines an asterisk may be part of a Hollerith string only when that string is surrounded by apostrohpes (e.g. 'X*Y') or defined by the nH convention (e.g. 3HX*Y). Similarly an apostrophe may be a part of a Hollerith string only when that string is surrounded by asterisks (e.g. *ED'S*) or defined by the nH convention (e.g. 4HED'S). On CDC machines (where FFORM currently does not recognize apostrophes) an asterisk may be part of a Hollerith string only when that string is defined by the nH convention.

When a single asterisk (or apostrophe) is encountered the remaining data on the card are treated as Hollerith data. This does not apply, of course, to an asterisk that is clearly a part of a Hollerith string.

When FFORM passes the data it has read to the calling program, it has stored Hollerith data six characters to the word. If the input description calls for one or more separate Hollerith words each word, therefore, must be six characters or less.

3.4.3 Implied Blanks and Zeroes

Pairs of commas, slashes, or left and right parentheses in consecutive columns of the card image will be interpreted as integer zeroes. Pairs of asterisks (or apostrophes) in consecutive columns of the card image imply Hollerith blanks.

e.g. ,, = () = // = 0
**** = '' = 1H

3.4.4 nR, the Repeat Option

nR causes the previous datum to be repeated n-1 times. n is an integer constant. When several pieces of data are enclosed by slashes or parentheses and are followed by a repeat instruction, the entire string of data will be repeated. Repeats can be nested by the use of slashes and parentheses, but each pair of symbols (// or ()) can be used only once per nest. This limits the depth of the nest to two levels.

e.g. 1.0,3R/2.0,1/2R = 1.0 1.0 1.0 2.0 1 2.0 1
/(WORD 2R) 3R/ 4R = WORD 24R

3.4.5 $, End of Card

All data including and following a $ will be ignored. This will permit the user to include comments on a card. The symbol $ between asterisks (or apostrophes) or somewhere in an nH field is not affected.

3.4.6 UNFORM and Card Type Numbers

Card type numbers must continue to appear in columns 1-2, but all subsequent data can be punched without regard to field definitions.

```
e.g.    UNFORM=A.NIP3
        01    title
        02    0 1 0 7R
             etc.
```

3.5 Microscopic Cross Sections - ISOTXS, XS.ISO and A.ISO

The binary CCCC interface file ISOTXS (see Appendix C.1) is the principal means for specifying microscopic cross section data for a DIF3D calculation. Users may alternatively supply either A.ISO, the formatted version of ISOTXS, or (at Argonne only) XS.ISO, the predecessor to ISOTXS at Argonne. Data from the alternative files are used to create a temporary ISOTXS file, the ultimate form in which data must be specified for use by DIF3D.

At Argonne, ISOTXS (and XS.ISO) files are generated by MC^2-2 (Ref. 38), a code which solves the neutron slowing down problem using basic neutron data derived from ENDF/B data files.[39] When XS.ISO is specified, an ISOTXS file is created by the module CSE010 early in the DIF3D Standard Path.

The formatted file, A.ISO, provides a machine independent means for exporting ISOTXS data. It also becomes ar expedient means for creating small cross section files for a variety of applications. The sample problem in Section 5.5.1 uses an A.ISO data set.

While creating an A.ISO data set special attention must be given to the fact that certain data records require an extra blank card-image. This requirement arises only when the number of data items is such that the portion of a format statement preceding a slash (/) is exhausted, but the portion following the slash is not used.

3.5.1 Reaction Versus Production Based (n,2n) Cross Sections

Users should be aware of at least two things about ISOTXS. First, in the principal cross-section record (also called the 5D record), there are slots for both transport and total cross sections. Cross-section sets generated by MC^2-2 (Ref. 38) contain both, and they are different. Second, there are slots for (n,2n) scattering cross sections in both the principal cross-section record and in the scattering sub-block record (the 7D record). The principal (n,2n) cross section, $\sigma_i^{n2n,g}$, is a vector of length equal to the number of energy groups. It is the probability, per unit group-g flux and per atom, that a neutron in group g will undergo an (n,2n) scattering reaction; i.e. it is reaction-based. The (n,2n) cross section in the 7D record, $\sigma_i^{g'g}(n,2n)$, is a group-to-group transfer matrix (number of groups by number of groups) which represents the probability that a neutron will be produced in group g' as a result of a scattering event in group g; it is production-based.

These definitions are clear in the current, version IV definition of ISOTXS found in Appendix C.1. There are notes at the end of the 4D record and 5D record that make the distinction and that point out that

$$\sigma_i^{n2n,g} = \frac{1}{2} \sum_{g'} \sigma_i^{g'g}(n,2n) \qquad (3.1)$$

Until about seven years ago, however, the file definition made no distinction between reaction-based and production-based cross sections, and there was a difference of interpretation within the FBR community.

Argonne previously used the XS.ISO format, in which elastic, inelastic and (n,2n) scattering cross sections were carried along in separate records. The (n,2n) reaction data was treated as being reaction-based. The practice was continued by storing reaction-based elastic, inelastic and (n,2n) scattering matrices separately in ISOTXS; our ISOTXS files normally do not contain a total scattering matrix. Most of the other FBR laboratories were used to dealing only with the total scattering cross section, and the factor of 2.0 (see Eq. (3.1)) required for the (n,2n) production-based matrix had to be factored into the total when the three partial reaction cross sections were summed. In other words, they were used to dealing with production-based cross sections. Due to this confusion it became necessary to tighten the definition in favor of the production-based interpretation, because a reaction-based, total scattering cross section is useless once the total has been formed - it is impossible to insert the factor of 2.0 that is needed in writing the scattering source term in the neutron balance equations. As a consequence of this inconsistency, HMG4C the code block which processes the microscopic data (ISOTXS) into macroscopic data (COMPXS) performs a check to determine whether the (n,2n) scattering matrix (if present) is reaction or production based. Hence the proper total scattering source is returned under either definition.

3.6 Number Densities, Cross Section Homogenization and Edits

The code block HMG4C combines microscopic cross sections (from ISOTXS) and atom number densities (from the CCCC files NDXSRF and ZNATDN) to form macroscopic cross sections. These macroscopic cross sections are output to a binary file called COMPXS (see Appendix D.1) which is read by DIF3D to obtain composition and energy group dependent data. HMG4C will optionally edit the COMPXS file contents.

3.6.1 Compositions, Zones and Subzones - A.NIP3 13 and 14 Cards

The terms composition and zone are used interchangeably in this report and in associated documentation. The term composition has traditionally been used at Argonne to mean a mixture of isotopes and a set of macroscopic cross sections. The term zone was introduced by the CCCC file definitions and is functionally equivalent to a composition. The definitions are not precisely the same, however. In the NDXSRF file there are volumes associated with zones - suggesting an additional, geometrical implication. This implied relation is never used by DIF3D. Each composition is simply assigned to one or more geometric regions of the reactor.

DIF3D provides the user with the means for creating several subcollections of isotopes so that the specification of isotopic mixtures may be simplified. This permits a building block approach whereby similar subcollections

(materials and/or secondary compositions) may be used in several compositions. The example supplied with the A.NIP3 file description (Appendix B.4) illustrates the flexibility provided by the A.NIP3 type 13 and 14 cards.

Materials can be defined on type 13 cards in terms of isotopes and/or in terms of other materials. Two types of compositions may be defined on the type 14 cards. Secondary compositions are mixtures of materials and/or isotopes. Primary compositions are mixtures of secondary compositions, materials and/or isotopes.

Materials do not exist in the CCCC environment, and the identity of individual materials is lost when the CCCC files NDXSRF and ZNATDN are created. Secondary compositions are treated as CCCC subzones. Those constituents of a primary composition which are not themselves subzones (i.e. isotopes and materials directly assigned to primary compositions) are combined into CCCC primary zone assignments.

The full generality of the NDXSRF file (see Appendix C.3) with regard to the specification of primary zone assignment volume fractions (VFPA(n)) and zone (and subzone) volumes is not, in fact, required by DIF3D. The input processing code block (GNIP4C) always assigns unity to VFPA(n) and the total volume occupied by all regions assigned to zone n is assigned to VOLZ(n). Each subzone volume (VLSA(m)) is chosen so that the ratio (VLSA(m)/VOLZ(n)) yields the volume fraction of subzone m computed from the type-14-card data. Factors on the type 13 or 14 cards other than subzone volume fractions (i.e. isotope atom densities and material volume fractions) are appropriately combined to form the atom density array (ADEN) on the ZNATDN file (see Appendix C.4). From this discussion we see that nowhere is the magnitude of VOLZ(n) and VLSA(m) critical; we only require their ratio.

3.6.2 Isotope Sets - A.NIP3 39 Cards

The concept of isotope sets is used to permit a reduction in the size of the CCCC atom density file (ZNATDN). All isotopes used in a particular zone or a particular subzone must be assigned to the same nuclide set. The default situation assigns all isotopes to the same set.

The size reduction occurs because of the nature of the matrix of atom densities stored on ZNATDN. The matrix is dimensioned NTZSZ x NNS (i.e. number of zones plus subzones x maximum number of nuclides in a set). Therefore, the introduction of two or more nuclide sets must reduce the dimension NNS.

3.6.3 Homogenization of Principal Cross Sections

The principal microscopic cross sections on the ISOTXS file are homogenized by the general formula

where

$$\Sigma_m^{x,g} = \sum_{i\epsilon m} \sigma_i^{x,g} n_{im} V_{im}^f \qquad (3.2)$$

$\Sigma_m^{x,g}$ is the macroscopic cross section of type x for energy group g and composition m;

$i\epsilon m$ denotes the set of isotopes assigned to composition m (via primary zone assignments and/or subzone assignments);

$\sigma_i^{x,g}$ denotes the linear combination of principal microscopic cross sections that define the type x macroscopic cross section (see Table 3.1);

n_{im} is the atom number density (ADEN on the ZNATDN file) assigned to isotope i in composition m;

V_{im}^f is the (primary zone assignment or subzone) volume fraction (on the NDXSRF file) associated with isotope i in composition m.

Table 3.1 summarizes the $\sigma_i^{x,g}$ assignments for all but the fission spectrum vector which is treated in Section 3.6.6. The scattering cross section homogenization also included in Table 3.1 is discussed in the next section. Several points regarding the removal cross section are noted in Section 3.6.5.

3.6.4 Homogenization of the Scattering Cross Section

The group g to g' scattering cross section $\sigma_i^{stot,g'g}$ can also be homogenized by Eq. (3.2) if we generalize the definition of $\sigma_i^{x,g}$ and $\Sigma_m^{x,g}$ (i.e. let $x \equiv stot,g'$). As shown in Table 3.1, the scattering cross section may be either in component form or in total form. The total scattering is defined by the linear combination of scattering components tabulated in Table 3.1. The factor f^{n2n} accounts for either reaction-based or production-based (n,2n) cross sections (see Section 3.5.1). If the macroscopic scattering matrix obeys the current ISOTXS rule and is production-based, this factor is unity. When that rule was imposed, however, Argonne had (and still has) cross section sets in which the scattering matrix was reaction-based. A factor of 2.0 was required for the homogenization of these cross sections. The solution of the problem was to code into the HMG4C module a test to see which form the cross section took. The following ratio is formed for each group that has (n,2n) scattering:

$$r^g = \sigma_i^{n2n,g} \Big/ \sum_{g'} \sigma_i^{g'g}(n,2n) \qquad (3.3)$$

where the principal (n,2n) macroscopic cross section is defined in footnote a of Table 3.1 (see also Eq. 3.1). If, for any group, this ratio is greater than .75, then $f^{n2n} = 2.0$. If this ratio is less than .75, $f^{n2n} = 1.0$ (Clearly, r should be .5 for production based data and 1.0 for reaction-based data). In this way HMG4C can detect whether the (n,2n) scattering matrix is reaction-based or production-based. At Argonne we continue to violate the production-based rule in ISOTXS files generated by MC^2-2, but HMG4C is able to handle both legal and illegal microscopic cross section sets.

In order to minimize storage on COMPXS, composition dependent maximum up- and down-scattering bandwidths (NUP_{gm} and NDN_{gm}) are calculated based on the maximum bandwidths of the isotopic constituents of the corresponding composition.

TABLE 3.1. Microscopic Cross Section Assignments to Macroscopic Cross Sections

Name	$\Sigma_m^{x,g}$	$\sigma_i^{x,g}$ assignments
Capture	$\Sigma_m^{c,g}$	$\sigma_i^{g}(n,\gamma) + \sigma_i^{g}(n,\alpha) + \sigma_i^{g}(n,p) + \sigma_i^{g}(n,d) + \sigma_i^{g}(n,t)$
Transport	$\Sigma_m^{tr,g}$	$\sigma_i^{tr,g}$
Total	$\Sigma_m^{t,g}$	$\sigma_i^{t,g}$
Fission	$\Sigma_m^{f,g}$	$\sigma_i^{g}(n,f)$
Removal	$\Sigma_m^{r,g}$	$\sigma_i^{c,g} + \sigma_i^{f,g} + \sum_{g' \neq g} \sigma_i^{stot,g'g} - \sigma_i^{n2n,g}$ [a]
Scattering	$\Sigma_m^{stot,g'g}$	$\begin{cases} \sigma_i^{elas,g'g} + \sigma_i^{inel,g'g} + f^{n2n}\,\sigma_i^{g'g}(n,2n) & \text{components}^c \\ \sigma_i^{stot,g'g} & \text{total}^c \end{cases}$
Power Conversion	PC_m^{g}	$E^{capt,g}\sigma_i^{c,g} + E^{fiss,g}\sigma_i^{f,g}$
Neutrons per Fission	$\nu\Sigma_m^{f,g}$	$\nu_i^{g}\sigma_i^{f,g}$
Fission Spectrum	χ_m^{g}	See Eq. (3.4) in text.

[a] $\sigma_i^{n2n,g} \equiv \frac{1}{2} f^{n2n} \sum_{g'} \sigma_i^{g'g}(n,2n)$. If $\sigma_i^{n2n,g}$ is absent from ISOTXS and the scattering matrices are in total-form, it is the user's responsibility to appropriately reduce (say) the capture cross sections.

[b] $b_f^{n2n} = \begin{cases} 1 & \text{production-based } \sigma_i^{g'g}(n,2n) \\ 2 & \text{reaction-based } \sigma_i^{g'g}(n,2n). \end{cases}$

[c] ISOTXS scattering data may be stored componentwise or in total form.

If higher order scattering cross sections are present in ISOTXS they will be ignored by HMG4C. The COMPXS file currently does not permit higher order scattering.

3.6.5 Discussion of the Removal Cross Section

The removal cross section accounts for two effects:

1. the loss of neutrons from the group due to absorption and outscatter;
2. the addition of neutrons to the group due to within-group (n,2n) scattering events.

The first two terms in the removal cross section definition in Table 3.1 represent losses of neutrons from absorption (i.e. from capture and fission). The last two terms represent the sum of the outscatter losses and the within group (n,2n) gain. Recall from Eq. (3.1) that the factor of .5 arises in the definition of $\sigma_i^{n2n,g}$ because the (n,2n) scattering matrix is production-based, and removal is reaction-based.

The presence of the principal cross section $\sigma_i^{n2n,g}$ in ISOTXS is optional. As noted in section 3.5.1 and Table 3.1 (footnote a), if data are expressed in total form with reaction-based (n,2n) cross sections, then it is impossible for HMG4C to determine the correct removal cross section. Consequently, it is up to the user to supply an ISOTXS file which accounts for the $\sigma_i^{n2n,g}$ effect in some other way. For example, one could reduce the capture cross section by the appropriate amount (a practice followed by at least one other laboratory).

3.6.6 Homogenization Options for the Fission Spectrum - A.HMG4C 02 Card

Any of three homogenization options are available by means of the prompt* fission spectrum flag. Denoting the fission fraction for group g of composition m by χ_m^g, then the options available for computing it are:

$$0 \ldots \chi_m^g = \bar{\chi}^g \tag{3.4a}$$

$$1 \ldots \chi_m^g = \frac{\sum_{i\epsilon m} \chi_{im}^g n_{im}^g V_{im}^f \sum_{g'} \nu_i^{g'} \sigma_i^{g'}(n,f)}{\sum_{i\epsilon m} n_{im} V_{im}^f \sum_{g'} \nu_i^{g'} \sigma_i^{g'}(n,f)} \tag{3.4b}$$

$$2 \ldots \chi_m^g = \frac{\sum_{i\epsilon m} \chi_i^g \nu_i^g n_{im} V_{im}^f \sigma_i^g(n,f)}{\sum_{i\epsilon m} \nu_i^g n_{im} V_{im}^f \sigma_i^g(n,f)}, \tag{3.4c}$$

*The issue of whether to compute a prompt or a total fission spectrum depends on the ISOTXS file supplied by the user. HMG4C simply uses the fission spectrum data as they exist on ISOTXS.

where the summation is over all isotopes i contained in composition m. $\bar{\chi}^g$ is the set fission fraction for group g while χ_i^g is the fission fraction for isotope i. The option 1 is termed total fission source weighting and may be derived from the expression for the fission source by assuming the flux is group independent. The option 2 is not recommended. In this option there is no assurance the χ_m^g summed over all groups will be unity for a given composition m.

Although the ISOTXS format permits the treatment of isotopic fission spectrum data which are incident energy dependent ($\chi_m^{gg'}$), neither the HMG4C nor the DIF3D code blocks can use such matrices. The weak energy dependence of the fission spectrum data in the LMFBR spectrum make it possible to use the vector derived at the average fission energy without any significant error.[40] The mixing of the different isotopic data to give a vector introduces a small error since the flux distribution is unknown, and assumed constant in the recommended algorithm. The algorithm does, however, account for the predominant isotopic effects so that the more rigorous matrix treatment is not warranted in view of the considerable data management costs which would result as a consequence of its use.

The presence on COMPXS of $\Sigma_m^{f,g}$ and χ_m^g data for composition m is indicated by the sentinel $ICHI_m$. $ICHI_m = 0$, indicates composition m is nonfissionable (i.e. composition m contains no isotopes with non-zero atom density that have a non-zero (n,f) cross section sentinel (IFIS) on the ISOTOPE-AND-GROUP-INDEPENDENT-DATA record of ISOTXS).

3.6.7 Edit Options and Container Storage - A.HMG4C 02 Card

Edit sentinels enable the user to direct edit output to either the print file (FT06F001) and/or an auxiliary file (FT10F001). HMG4C error messages, however, will appear only on the print file. Both the COMPXS (including a user supplied COMPXS) and the ISOTXS files may be edited. The ISOTXS edit is a running edit of those isotopes referenced in the homogenization.

The computer resource requirements (both container storage and CPU time) of the HMG4C code block are insignificant compared to the typical requirements of the DIF3D (neutronics solution) code block. Therefore, the user need only supply a main (FCM) memory size on the A.HMG4C type 02 card that is less than or equal to the sum of the FCM and ECM sizes on the A.DIF3D type 02 card. On two-level machines, of which the CDC 7600 is the only pertinent example, the FCM size from DIF3D is a reasonable estimate. It should be noted that the HMG4C FCM container size may also be specified on the A.NIP3 type 02 card. If both specifications are present, the A.HMG4C specification takes precedence.

In computing the homogenized cross sections, the code attempts to hold as much of the macroscopic cross section data in memory as the container space will permit. If all the macroscopic data will not fit in the available memory, the code determines the maximum number (m) of compositions which can be accomodated in a single pass. As many passes are then made as required to homogenize all the compositions. Taking this multipass mode of operation to the extreme, just one composition may be computed in each pass. Since there

are a total of NZONE compositions to be formed (one for each ZONE in the problem), the expression for the main (FCM) storage requirement is of the form,

$$FCM = A + mB, \quad 1 \le m \le NZONE,$$

where A is the amount of storage required to hold the microscopic data and B is the amount needed to hold the macroscopic arrays for a single composition.

HMG4C always prints the actual number of words used and, if in multipass mode, the number of words required for a single composition and the number of passes to be used. These data may then be used as a guide for subsequent runs.

3.6.8 Directional Diffusion Coefficient Factors - A.NIP3 35 and 36 Cards

DIF3D will generate directional diffusion coeffficients of the form

$$D_m^{n,g} = A_m^{n,g} * D_m^g + B_m^{n,g}, \quad n=1,2,3, \tag{3.5}$$

using factors $A_m^{n,g}$ and $B_m^{n,g}$ specified on the A.NIP3 35 and 36 cards. The code block MODCXS writes these factors into COMPXS after HMG4C has completed the homogenizations.

The calculation of transverse leakage by DIF3D always uses the third dimension diffusion coefficient $D_m^{3,g}$ for the pseudo absorption

$$(DB^2)_m^g = D_m^{3,g} * (B_m^2)^g \tag{3.6}$$

used on option regardless of the problem dimension. The composition-dependent buckling $(B_m^2)^g$ is discussed in Section 3.75 and defined in Eq. (3.26) of Section 3.14.7.

3.6.9 Fission and Capture Energy Conversion Factor Data - A.NIP3 37 and 38 Cards

Fission and capture energy conversion factors (E_m^{capt} and E_m^{fiss}) in the ISOTXS file may be overridden for particular compositions by supplying the appropriate data on the A.NIP3 type 37 and 38 cards - units are fissions per watt-second and captures per watt-second, respectively.

3.7 Geometry Input and Edits - A.NIP3 and GEODST

The primary means of specifying the model geometry for a DIF3D calculation is the A.NIP3 DATASET. The card-by-card input description is given in Appendix B.4. As of the date of this report there are 43 card types in A.NIP3, 16 of which (02-12, 15, 29-34 and 43) can be used to define and edit the geometry. Of these 16 fewer than half are usually required to define a model.

The alternative to the geometry description cards in A.NIP3 is the CCCC Standard Interface File GEODST. Its file description is included in Appendix C.2.

The code block GNIP4C reads A.NIP3 (if it is input) and writes a GEODST file. GNIP4C also produces an edit of the geometry.

3.7.1 Geometry Types - A.NIP3 03 Card

The only datum on the A.NIP3 03 card is the geometry type sentinel. Geometry types currently implemented in the DIF3D finite-difference solution algorithms are:

Slab (10)
Cylinder (20)
X-Y (40) and X-Y-Z (44)
R-Z (50)
Theta-R (64) and Theta-R-Z (66)
Triangular (70) and Triangular-Z (90), rhombic region of solution, core center at 60 degree angle (sixth-core symmetry).
Triangular (72) and Triangular-Z (92), rectangular region of solution (half-core symmetry).
Triangular (74) and Triangular-Z (94), rhombic region of solution, core center at 120 degree angle (third-core symmetry).
Triangular (78) and Triangular-Z (98), rectangular region of solution (quarter-core symmetry).
Triangular (80) and Triangular-Z (100), rectangular region of solution (full core).

The numbers in parentheses are the A.NIP3 type 03 card geometry sentinels. The input processor GNIP4C will actually accept and correctly process the additional geometry sentinels:

Spherical (30)
R-θ (60) and R-θ-Z (62)
Hexagonal with full (110), sixth (114) and third (116) core symetries
Hexagonal-Z with full (120), sixth (124) and third (126) core symetries.

The DIF3D nodal option[5] solves the hexagonal geometry options.

3.7.2 Boundary Conditions - A.NIP3 04, 05, 10, 11 and 31 Cards

External boundary conditions types are defined on the type 04 card. Boundary conditions permitted by the DIF3D finite-difference solution option are:

Zero flux (2)
Zero gradient (3)
Extrapolated (4) ($D \cdot \phi' + A \cdot \phi = 0$)
Periodic (6), with opposite face (X-direction only)
Periodic (7), along the adjacent boundaries meeting at the origin.

GNIP4C will process additional, periodic and transport-theory boundary conditions, but the DIF3D code block will not accept them.

The constants required by the extrapolated condition are input on the 05 card. Internal, blackness-theory boundary conditions and constants are defined on the type 10 and 11 cards. Type 05, 10 and 11 cards may be omitted when they are not required.

For triangular mesh geometries it is possible to reduce the region of solution by not defining a background region (the type 31 card). This yields a region of solution outer boundary which can follow the irregular shape of an outer ring of hexagons. Whenever DIF3D detects an irregular boundary situation, it determines a single boundary condition from the user-specified boundary conditions and applies it to all external mesh surfaces that do not coincide with the parallelogram or rectangular envelope of the region of solution. If more than one type of boundary condition is specified, the zero flux condition takes precedence; the extrapolated condition is next in rank, and the zero-current condition is least in rank.

Physical considerations strongly reinforce the recommendation that boundary condition specifications along the irregular outer boundary should be uniformly specified. Therefore, it is recommended that the boundary condition specifications for all X- and Y-direction surfaces which are not symmetric (zero-current) or periodic in nature, be identically specified (e.g. zero-flux or extrapolated, but not both)!

3.7.3 Regions and Areas - A.NIP3 06, 07, 15, 30 and 31 Cards

Regions are geometrical shapes, bounded by mesh lines, that contain a homogeneous composition. For orthogonal geometries (e.g. X-Y-Z, R-Z) regions are defined on the 06 cards. For triangular and hexagonal geometry models regions are defined in terms of concentric rings of hexagons on the type 30 cards. A region name for the background region, all the mesh cells outside the hexagons defined on type 30 cards, is defined on the 31 card.

Areas are collections of possibly non-contiguous regions. They are a convenience provided for input and editing and are defined on the type 07 card.

The correspondence between regions (or areas) and the compositions they contain is made on the type 15 cards.

3.7.4 Mesh-Spacing - A.NIP3 06, 09 and 29 Cards

The 1st dimension and 2nd dimension mesh for orthogonal geometry models can be defined on either the 06 or 09 cards. The 3rd dimension (Z) mesh is always defined on 09 cards. The mesh size for triangular mesh geometries is determined from the hexagon flat-to-flat distance input on the 29 card.

3.7.5 Bucklings - A.NIP3 12 and 34 Cards

Bucklings can be specified by composition and group on the type 34 cards.

Alternatively, the user can input a transverse half height on the type 12 card which is used to calculate a group-independent buckling and which is also used as a transverse finite dimension for flux and power integrals. Users should read the 12 and 34 card input descriptions for a discussion of what happens when both 12 and 34 cards are input. Section 3.14.2 discusses the impact of the type 12 and 34 cards on the edits of the flux integrals.

3.7.6 Geometry Edits - A.NIP3 02 and 43, A.DIF3D 04 Cards

Printer edits of the geometry may be turned on by means of sentinels on the type 02 card of A.NIP3 and the 04 card of A.DIF3D. These two edits include substantially the same data, but in different formats.

Graphics (e.g. CALCOMP) maps of the geometry for two- and three-dimensional models can be produced by setting a flag on the type 43 card. At Argonne the user must invoke the POSTPLOT procedure to direct the graphics output to the desired device. The graphics output may not be available in all export versions of the code (see Section 4.1.5).

3.8 Distributed, Inhomogeneous Sources - A.NIP3, FIXSRC and A.DIF3D

DIF3D will accept any kind of distributed, inhomogeneous source if it is input in the CCCC Standard Interface File FIXSRC (see Appendix C.5). DIF3D will not accept inhomogeneous boundary sources. On short-word machines the FIXSRC file DIF3D expects (and which the GNIP4C code block optionally provides) violates the CCCC standards in one respect; the source distribution must be given in REAL*8 words, rather than REAL*4 words. FIXSRC sources for adjoint problems must be stored in reverse group order, as in the ATFLUX file.

Inhomogeneous source problems are indicated to DIF3D via a sentinel specified on the type 03 card of A.DIF3D. The type 08 card of A.DIF3D evokes the alternate outer-iteration acceleration strategy discussed in Section 2.2.8; a single asymptotic extrapolation precedes the application of the conventional, Chebyshev semi-iterative acceleration strategy.

The BCD input processor GNIP4C will generate three special types of fixed sources from data on one or more of four A.NIP3 cards (19 and 40-42).

3.8.1 By Group, By Region or Mesh - A.NIP3 19 Cards

Fixed source densities can be input on A.NIP3 type 19 cards by combinations of group, region and mesh. This is an efficient way of doing it when a few regions or mesh cells are to contain a constant source density, but it becomes tedious if the source density extends over a large number of mesh and is mesh and group dependent.

3.8.2 Synthesis Trial Function Source - A.NIP3 40 Card

In flux-synthesis calculations it is sometimes helpful to have trial functions which represent axial blanket or reflector zones and which come from fixed source calculations. The fixed source is the pointwise product of a group flux from some other calculation and the local diffusion coefficient. GNIP4C will prepare such a source given an input RTFLUX file and the proper flag on the A.NIP3 type 40 card. The user should be aware that DIF3D will overwrite the input RTFLUX with the flux solution from the fixed source problem.

3.8.3 Natural Decay Source - A.NIP3 41 and 42 Cards

GNIP4C will generate a distributed source which is the product of an isotope decay constant, the isotope number density and an isotope spectrum (or sums of such products) by mesh and group. Isotope names and decay constants are specified on type 41 cards, the number densities from other input (the type 13 and 14 cards or the ZNATDN file) and the spectra from type 42 cards.

3.8.4 Source Edits - A.NIP3 40 Card

An edit of the fixed source file (either generated from A.NIP3 input or input via FIXSRC directly) may be obtained by turning on the edit sentinel on the type 40 card. The source edits may be sent to either or both of the edit files.

3.9 Code Dependent Input - A.DIF3D

DIF3D calculational parameters, storage containers and edit sentinels are specified via the A.DIF3D DATASET. The card-by-card description of A.DIF3D is found in APPENDIX B.1.

The alternative to data specification via A.DIF3D is the binary interface file named DIF3D (not to be confused with the module DIF3D). Its file description is provided in Appendix D.2.

The code block BCDINP reads A.DIF3D and writes the interface file DIF3D. If A.DIF3D does not exist, BCDINP writes the DIF3D file using default data. If both A.DIF3D and DIF3D exist BCDINP reads both files. Data existing in the DIF3D file will be overwritten only by its non-zero and non-blank counterparts in the A.DIF3D data set (i.e. defaulted datum fields cannot overwrite their counterparts on the DIF3D file). Consequently, it is a good habit to avoid explicit specification of default data so that recently updated parameters on the DIF3D file are not reset to the default values in subsequent restart jobs.

3.9.1 Data Management Options and Container Sizes - A.DIF3D 02 Card

The DIF3D data management strategy accomodates a wide variety of problems on computers with differing architectures. The key feature of this strategy is that it employs a fast core memory (FCM) container and an extended core memory (ECM) container to optimize the storage utilization on both one-level and two-level storage hierarchy machines in a unified manner (See Section 4.3). The two containers reside in separate memory levels on two-level machines (e.g. SCM and LCM on the CDC 7600). Both containers reside in main storage on single hierarchy machines (e.g. IBM 370/195).

Major scratch file buffers (also called ECM files) for the flux, finite-difference coefficients and cross section files reside in the ECM container. Files that cannot be contained in ECM, require random access I/O transfers between ECM and their peripheral storage devices.

The FCM container contains miscellaneous arrays required for input processing and several arrays (with lengths on the order of the number of mesh intervals in a mesh line) required during the steady state flux calculation.

On two-level machines additional FCM container space is required for buffering one group of cross sections and blocks of mesh lines in a plane between ECM and FCM for efficient computation in FCM (see Section 4.3.2.3).

DIF3D invokes one of several storage strategies based on the user specified FCM and ECM container sizes. On two-level machines the FCM block sizes range from full plane blocking to partial plane blocking with a minimum of one mesh line per block.

Except for three-dimensional problems, one group of fluxes, finite-difference coefficients and composition cross sections along with three group-independent source arrays and a mesh-interval-to-composition map array

are the minimum data that must be contained in ECM. If the available ECM exceeds this minimum, DIF3D first attempts to ECM-contain a scattering band of fluxes and then any of the remaining files.

Large three-dimensional problems may require the concurrent inner iteration strategy (CIIS). It requires that data for only a subset of the total number of mesh planes be contained in ECM during the inner iterations for an energy group. In this mode an unlimited number of mesh planes is permitted with limitations only on the number of mesh cells in the plane.

The strategies just summarized permit the user to vary the computer resource requirements to suit specific needs for a particular job. Three resources are primarily affected by the choice of container size. They include core storage, disk storage and I/O processing units (called EXCP's on IBM systems or Peripheral Processor (PP) time on CDC systems). It is usually preferable to ECM-contain the maximum amount of data to avoid excessive I/O charges. On systems where I/O charges are negligible or when excessively high core storage requirements inhibit job turnaround time users may choose to incur the additional I/O activity so that earlier job scheduling is obtained.

Users who wish to devote little time to data management considerations are urged to supply as large an ECM container size as possible since it is usually cheaper to overestimate the required ECM storage size than it is to underestimate ECM and incur the resulting excessive I/O charges.

Formulas for calculating the minimum FCM and ECM container sizes for one- or two-level machines are displayed in Table 3.2. The minimum ECM size estimate for the CIIS is provided primarily to indicate the relative storage requirements of the problem. Every effort should be made to avoid running problems at this minimum ECM size to avoid an enormous I/O overhead. In extreme cases job costs can be more than tripled!

A summary of the DIF3D storage allocation parameters is edited with every DIF3D problem. Figure 3.2 illustrates a data management summary page that may be obtained for Sample Problem 4. Edits of the minimum number of words required to run the problem in each data management mode provide the user with the necessary information to determine the feasibility of running a problem with a more efficient strategy. Also included is a tabulation of the location, size and associated record lengths of the principal random access (DOPC) files. In the two-level implementation an edit of the number of lines per plane contained in FCM is also indicated.

In three-dimensional problems the data management page includes an edit of the minimum data required for the CIIS. If the CIIS strategy is invoked, the number of planes in a record (or block), the number of records to be simultaneously contained in ECM and the number of container words in a block of planes is edited. The latter data are sufficient to determine the ECM container size adjustments needed to achieve a given inner iteration bandwidth.

It is possible to obtain just the data management edit page, so as to optimize the container size estimates prior to performing the desired neutronics calculation. This may be accomplished by supplying a ridiculously small ECM container size (say two words) which causes DIF3D to terminate abnormally after printing the data management page.

TABLE 3.2. A.DIF3D FCM and ECM Minimum Container Size Estimation

Parameters

I,J,K = Number of 1-, 2-, and 3-D mesh intervals
NRING = Number of hex rings in triangular geometry
NDIM = Number of problem dimensions (1,2 or 3)
NCELLS = Number of spatial mesh cells (I*J*K)
NGROUP = Number of energy groups
MAXSCT = Maximum scattering bandwidth
NCMP = Number of compositions (zones)
NCXS1G = Storage for 1 group of cross section data
= (9+MAXSCT)*NCMP
LDW = Word length parameter
= (1 on longword, 2 on shortword machines)

Triangular Geometry I and J Estimates

I	J	Symmetry Option
6*NRING-1	4*NRING-2	Full Core
6*NRING-1	2*NRING-1	Half Core
2*J	2*NRING-1	Third Core
3*NRING	2*NRING-1	Quarter Core
2*J	(3*NRING-1)/2	Sixth Core

Minimum Storage Size Estimates	Application
FCM = NCXS1G + 12*I*J	2-level full plane[a]
FCM = NCXS1G + 19*I	2-level partial plane[a]
FCM = MAX(1500, 15*MAX(I,J), (15+MAXSCT)*NGROUP)	1-level[b]
ECM = NCXS1G + (8+1./LDW)*NCELLS + I*J	1 group in core
ECM = NCXS1G + (23+1./LDW)*I*J	Concurrent Inner Iteration Strategy

[a]2-level storage hierarchy machines such as CDC 7600.
[b]1-level storage hierarchy machines such as IBM 370 systems.

*** DIF3D STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	600	75000
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH 3 PLANES FOR 1 GROUP IN CORE	=	508	12225
WITH ALL DATA FOR 1 GROUP IN CORE	=	508	152345
WITH SCATTERING BAND OF FLUXES IN CORE	=	508	205913
WITH ALL FILES IN CORE	=	508	438257

LOCATION OF SCRATCH FILES DURING STEADY STATE CALCULATION

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NEW FISSION SOURCE	8	2480	17856	DISK	1
OLD FISSION SRC. 1	8	2480	17856	DISK	1
OLD FISSION SRC. 2	8	2480	17856	DISK	1
TOTAL SOURCE	8	2480	17856	DISK	4
COMPOSITION MAP	8	1240	8928	DISK	1
FLUX ITERATE	32	2480	71424	DISK	6
CROSS SECTIONS	4	72	288	CORE	4
FINITEDIFF. COEFS.	32	9920	285696	DISK	4

PROBLEM WILL BE RUN WITH AN EFFECTIVE BANDWIDTH OF 2 RECORDS WITH 5 PLANES/RECORD YIELDING 10 INNER ITERATIONS/CONCURRENT ITERATION PASS. THE NUMBER OF ECM CONTAINER WORDS REQUIRED TO INCREMENT OR DECREMENT THE INNER ITERATION BANDWIDTH BY 5 INNER ITERATIONS IS 14880 WORDS PROVIDED THE CURRENT BLOCK LENGTH IS MAINTAINED.
(I.E. ENTER THE BLOCK LENGTH 2480 IN COLS. 25-30 OF THE A.DIF3D TYPE 03 CARD).

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM	=	508	73945

Fig. 3.2. A Data Management Page Edit for Sample Problem 4

3.9.2 Solution Options and Control Parameters - A.DIF3D 03 Card

Parameters supplied on the type 03 card of A.DIF3D select the problem type (criticality or distributed inhomogeneous source) and the solution type (real or adjoint). Outer iteration control parameters which limit the maximum number of outer iterations, and optionally override the Chebyshev acceleration of the outers are also present. The outer iteration limit can be used to bypass the outers entirely and simply obtain selected integral edits. In large problems requiring one or more restarts it is economical to request the integral edits only after convergence is achieved.

Two parameters on this card are related to the concurrent inner iteration strategy (CIIS) which is invoked in large three-dimensional problems whenever the ECM container storage is insufficient for the one-group-in-core strategy (see Section 3.9.1). The first parameter is the minimum record size (MINBSZ) in long words for the I/O transfer of blocks of planes in the CIIS. The default values were chosen in an attempt to balance I/O overhead with the ECM storage overhead incurred as the size of the blocks of planes increases (see Section 3.10). The other parameter, the CIIS efficiency factor, avoids the last pass of inner iterations in those groups for which the number of inner iterations falls below a code-dependent threshold. The following simple example illustrates the point: suppose a bandwidth of 12 inner iterations can be performed in a single concurrent iteration I/O pass across the group-dependent data. If in a particular group the required number of inners/outer (m_g) is 13, then the second I/O pass required to perform the single remaining inner iteration is scarcely cost effective.

Problems with thermal scattering frequently require upscatter iterations to ensure convergence. The number of such upscatter iterations performed in every outer is specified on the type 03 card if the default value of 5 upscatter iterations per outer iteration is inappropriate.

The job time limit entry on the type 03 card of A.DIF3D is intended to force graceful termination (i.e. to ensure that restart files - RTFLUX and DIF3D - are saved) on those systems in which the amount of CPU time remaining is not an available quantity to subroutine TIMER. To prevent job failures due to time limit, the user must specify a time limit on the type 03 card which is sufficiently less than the job time limit to permit DIF3D to trigger a graceful termination based on the elapsed time clock.

3.9.3 Convergence Criteria - A.DIF3D 05 and 06 Cards

Three outer iteration convergence criteria (Eqs. 2.89 - 2.91) are supplied on the type 05 card of A.DIF3D:

1. Absolute eigenvalue change, ε_k;
2. Pointwise fission source error, ε_λ;
3. Average relative fission source error, ε_ϕ.

All criteria must be satisfied before the outer iterations are converged. When the default convergence criteria are used, the pointwise fission source convergence is typically the last criterion satisfied.

Only one parameter related to the inner iteration convergence can be specified by the user and it is on the type 06 card of A.DIF3D. This parameter specifies the error reduction factor to be achieved by each series of inner iterations for each group during each outer iteration of the calculation. Prior to the start of the outer iterations this factor is used along with the precalculated optimum overrelaxation factors to compute the number of inner iterations required in each group. Experience has shown that this parameter provides an effective means for ensuring uniform convergence behavior.

Included in the edits of every DIF3D problem will be the precalculated optimum overrelaxation factors and an iteration history in which the fission source and k-effective convergence are tabulated. Figure 3.3 illustrates the outer iteration history page from Sample Problem 1.

3.9.4 Edit Options and Interface File Output - A.DIF3D 04 Card

The first four of the eleven edit options on the type 04 card of A.DIF3D simply provide edits of various input quantities and all but the first have already been discussed in their respective applications. Key dimensions for geometry and cross section data are edited along with boundary conditions, zone bucklings, mesh interval data and region to zone assignments.

Certain data are always edited. Included in this category are the data specified on the A.DIF3D file, the DIF3D data management page (a summary of storage allocation options), lists of interface files read or written, the outer iteration history, the optimum overrelaxation factors by group, and a computing time summary which tabulates computation times by each logical computation section in DIF3D.

Edit options five through nine provide integrals by region, region and group, and by group for neutron balance, power distribution and flux distribution. Except for the neutron balance these items are also available by mesh cell. All but power distribution data are available also for adjoint problems.

The mesh cell and energy dependent flux interface file RTFLUX (ATFLUX in adjoint problems) is always written upon termination of the outer iterations. The power-density-distribution-by-mesh-cell interface file PWDINT and the zone-averaged flux file RZFLUX can be optionally written in real problems by specifying edit option ten.

DIF3D provides edits of commonly expected integral quantities. All requested edits that are not also written to one of the CCCC interface files are written to the code-dependent interface file D3EDIT. Section 3.14 defines these edit quantities.

Some users find it useful to obtain additional edits appropriate to their applications by writing programs which manipulate data available on the various interface files described in this document. The UDOIT1 - UDOIT4 modules discussed in Section 4.1.11 are appropriate for this application.

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS
1	1.42092D+00	7	2	1.57656D+00	11	3	1.27169D+00	5	4	1.26615D+00	5

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
1	6.055469D-01	1.686693D-01	5.676263D-02	0	0.0	0.0	1.05676263D+00
2	4.704232D-01	1.306399D-01	3.391310D-02	0	0.0	8.269922D-01	1.09067574D+00
3	1.767146D-01	7.337978D-02	1.908419D-02	0	0.0	5.957153D-01	1.10975993D+00
4	8.690130D-02	4.552007D-02	8.680460D-03	1	5.957153D-01	5.957153D-01	1.11844039D+00
5	3.722962D-02	2.073863D-02	5.107754D-03	2	5.957153D-01	6.254009D-01	1.12354814D+00
6	1.064050D-02	6.314254D-03	2.468417D-03	3	5.957153D-01	6.280142D-01	1.12601656D+00
7	3.829818D-03	2.197660D-03	8.781398D-04	1	6.280142D-01	6.280142D-01	1.12689470D+00
8	1.806451D-03	1.012883D-03	2.399321D-04	2	6.280142D-01	6.305913D-01	1.12713463D+00
9	4.606560D-04	2.320342D-04	9.278793D-05	3	6.280142D-01	6.203958D-01	1.12722742D+00
10	1.203257D-04	7.173725D-05	3.893697D-05	4	6.280142D-01	6.331385D-01	1.12726635D+00
11	2.823481D-05	1.472779D-05	1.050205D-05	1	6.331385D-01	6.331385D-01	1.12727686D+00
12	1.556538D-05	1.031790D-05	2.427902D-06	2	6.331385D-01	7.953652D-01	1.12727928D+00
13	4.066891D-06	1.710762D-06	7.286502D-07	3	6.331385D-01	6.304855D-01	1.12728001D+00
14	9.684399D-07	7.739674D-07	3.097159D-07	4	6.331385D-01	6.577679D-01	1.12728032D+00
15	2.049522D-07	1.272518D-07	8.601389D-08	1	6.577679D-01	6.577679D-01	1.12728041D+00

OUTER ITERATIONS COMPLETED AT ITERATION 15, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.12728040833

TO RESTART THIS CALCULATION, INPUT FOLLOWING VALUES

DOMINANCE RATIO (SIGBAR) = 6.577679231397D-01

OPTIMIZED OVER-RELAXATION FACTORS

GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA
1	1.42092D+00	2	1.57656D+00	3	1.27169D+00	4	1.26615D+00		

MAXIMUM POWER DENSITY 2.68379D-04 OCCURS AT MESH CELL (I,J,K) = (1, 1, 1)

PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX VALUES ON THE CELL SURFACES AND WITHIN THE CELL.

Fig. 3.3. Iteration History Page Edit for Sample Problem 1.

3.9.5 Restart Option - A.DIF3D 03, 06 and 07 Cards

Restart jobs generally differ from the original job in two ways. The appropriate flux DATASET (RTFLUX or ATFLUX) must be provided and specified under "BLOCK=OLD" in the BCD input data. Appropriate JCL designations are required to ensure that the system accesses the appropriate restart flux file. Optimum overrelaxation factors and the latest eigenvalue and dominance ratio estimates should also be provided. The most convenient means for specifying the last three items is to supply the restart file DIF3D and specify it under "BLOCK=OLD". Note that the restart sentinel will already be set on the DIF3D file if the file was written by a job in which outer iteration convergence was not achieved. An alternative is to revise the original A.DIF3D file by specifying the above data on card types 06 and 07 and by specifying the restart sentinel on the type 03 card.

The precalculation of optimum overrelaxation factors generally requires CPU time equivalent to two or three outer iterations, so that it is well worth the effort in problem restarts to supply these factors. The remaining factors supplied during restarts facilitate resumption of the Chebyshev fission source acceleration with minimal loss of efficiency. In applications in which a series of related problems are to be solved the optimum overrelaxation factors frequently are quite similar. Consequently the optimum overrelaxation factors for a common set of problems may be calculated once in the first problem of the set and used throughout.

3.9.6 Acceleration of Near-Critical Source Problems - A.DIF3D 08 Card

An optional strategy which accelerates the outer iteration convergence in near-critical systems with an inhomogeneous source (see Section 2.2.8) can be invoked by specifying the appropriate data on the type 08 card of A.DIF3D. The strategy provides more rapid convergence for this class of problems than the Chebyshev acceleration techniques generally applied to most DIF3D problems.

3.9.7 Neutron Transport Option - A.DIF3D 09 Card

At Argonne there exists a version of DIF3D in which the diffusion theory inner iteration routines have been replaced by a transport theory (Sn) calculation. As of the date of this report there were no plans to make a formal release of DIF3D/transport to any code centers.

One invokes DIF3D/transport in the Argonne system by including

```
PRELIB='C116.B99983.MODLIB'
```

on the EXEC card for STP021. The type 09 card of A.DIF3D specifies the transport option. It contains the S_n order as well as the control parameters for the innermost line-sweep iteration.

3.10 Guidelines for the Efficient Use of the CIIS

Typical problems invoking the Concurrent Inner Iteration Strategy (CIIS) (see Section 4.3.2.2) make heavy demands on computing system resources including:

1. CPU Time,

2. I/O Processor Time (EXCP's on IBM systems),

3. Central Memory Storage (FCM and ECM),

4. Disk Storage.

Items (1) and (4) are essentially invariant for a given problem, while items (2) and (3) are dependent on the ECM storage container size. Item (2) is also dependent on MINBSZ, the desired I/O record size (see Section 3.9.2). Within practical limits, resources (2) and (3) are roughly inversely proportional, so that as the ECM size increases, the inner iteration bandwidth B increases, yielding a corresponding decrease in the number of inner iteration I/O passes and vice versa. This flexibility in resource allocation afforded by the range of permissible ECM values enables the user to tailor the resource utilization for an arbitrary problem to an arbitrary host installation.

3.10.1 Optimal ECM Size Estimation - A.DIF3D 02 Card

If a reasonable estimate exists for M, the average number of inner iterations per outer iteration required for the problem at hand, then the procedure below determines the least storage needed to minimize the number of inner iteration I/O passes having block size MINBSZ. For example, if M=24 in a given problem but the maximum ECM-containable inner iteration bandwidth B is B=18, then the algorithm will choose U, the number of ECM-contained I/O blocks, and L, the number of planes in an I/O block, such that $B=U \cdot L \geq 12$. A bandwidth of 12 iterations requires the least ECM storage to perform the inner iterations in two I/O passes.

The four-step procedure detailed below, provides simple guidelines for users to obtain a quick estimation of the appropriate ECM container size for a problem that may need the CIIS option. Formulas and parameter definitions are tabulated in Table 3.3 for short-word and long-word machines and for machines with one- or two-level storage hierarchies. Figure 3.4 graphically depicts ECM storage requirements W(U,L) as a function of the number of ECM-contained blocks U for blocks ranging in size from L=1 to L=15 planes. Constant bandwidth (dashed) curves, $B=U \cdot L$, B=5,10,...,50 are also plotted to clearly indicate the relative storage overhead incurred as the block size L is increased.

The ECM estimation procedure is given by the following four steps:

Step 1: Determine the maximum container space available for the variable size plane-block arrays,

$$WMAX = (\min (ECMMAX, ECM1G) - ECMISC) / (IM*JM) .$$

WMAX is limited by either the machine dependent maximum ECM size (ECMMAX) or by the minimum container size (ECM1G) for the one-group contained data management option.

TABLE 3.3. ECM Size Estimation for the CIIS

Parameter Definitions[a]

M	=	Maximum number of inner iterations (m_g) per outer in any group.
BLMAX	=	Maximum ECM system buffer length (usually 32768).[b]
INDEXR	=	ECM space required for dynamic random access I/O index in XCM.
MACHUPE[c]	=	3000K bytes on the IBM 370/195 at ANL.
	=	8000K bytes on the IBM 3033's at ANL.
	=	393216 LCM words on the CDC 7600 at LBL.
	=	294912 words of LCM on the CDC 7600 at BNL.
MACHUPF[c]	=	61440 words of SCM on the CDC 7600.
PROGSIZE	=	Memory required to contain longest overlay in DIF3D.
ECMISC	=	(9+MAXSCT)*NCMP+I*J
ECMMAX	=	MACHUPE-FCM-PROGSIZE on the IBM 370/195. MACHUPE-FCM-PROGSIZE-BLMAX-INDEXR(L) on the CDC 7600.
ECM1G	=	ECMISC+(8+1/LDW)*NCELLS
INDEXR(L)	=	Q(L)*(5*NGROUP+9) + NGROUP
Q(L)	=	(K-1)/L+1
W(U,L)	=	(min(U+2, Q(L))*5 + min(U+3, Q(L)) + 4.5)*L

ECM Estimation Algorithm Summary

1) WMAX	=	(min (ECMMAX, ECM1G) - ECMISC) / (IM*JM)
2) L	=	min (MINBSZ/(I*J)+.5, K, WMAX/W(1,1))
3a) U	=	max U subject to W(U,L)<WMAX (graphical estimate Fig. 3.4.)
3b) P	=	(M-1)/(L*U) + 1
3c) U	=	(M-1)/P + 1
4)ECMCC	=	ECMISC + W(U,L)*I*J

[a]See Table 3.2 for additional parameter definitions.

[b]On the LBL system default system buffer sizes are overridden by the FBSIZE and GBSIZE control cards.

[c]MACHUPn is the estimated maximum storage available to the user for the ECM container (n=E) or FCM container (n=F).

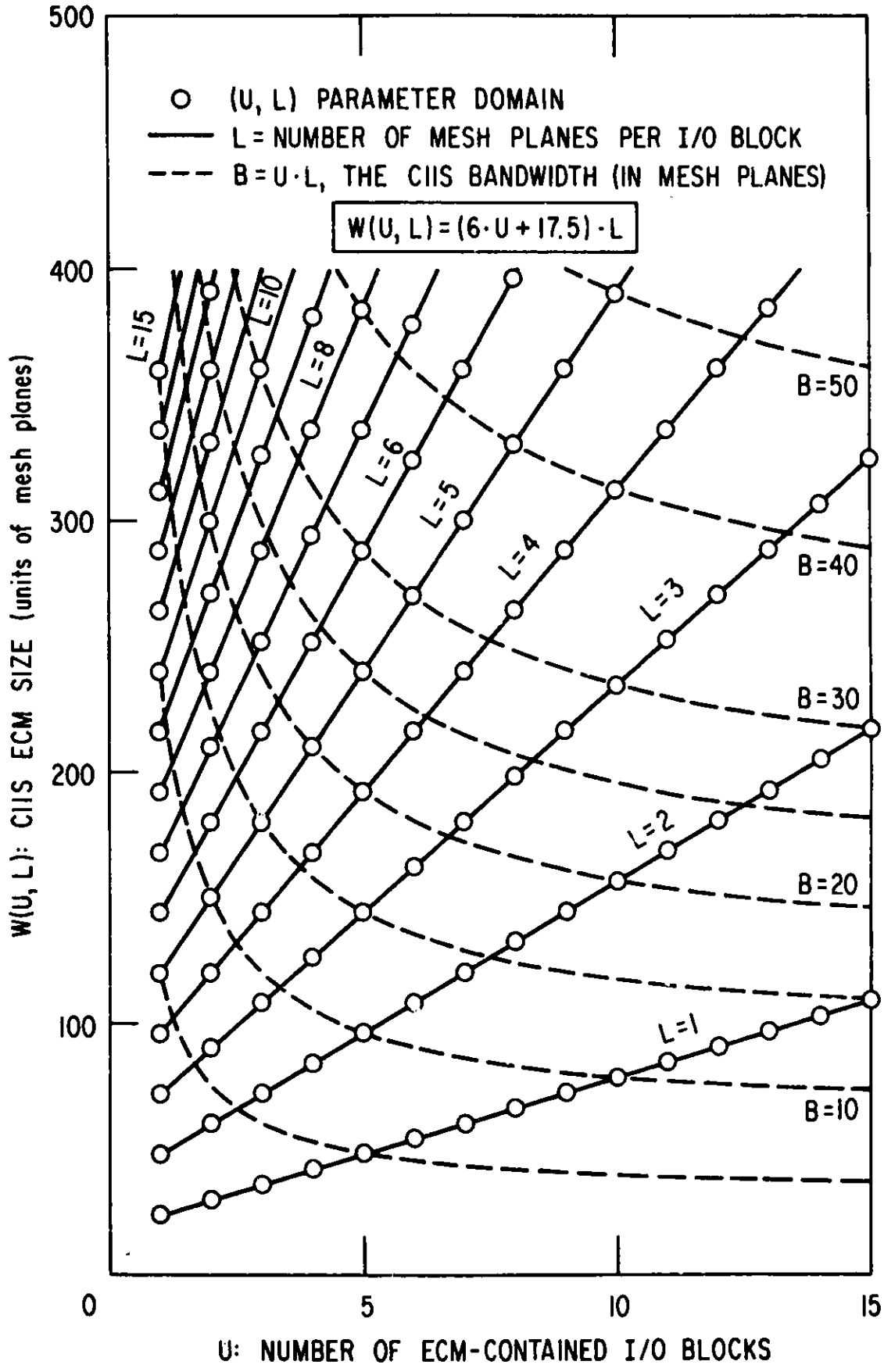

Fig. 3.4. CIIS ECM Storage Requirements Guide

Step 2: Determine L, the near-optimal number of planes in a block

L = min(MINBSZ/(I*J)+.5, K, WMAX/W(1,1)) .

L cannot exceed the number of planes (K) in the problem or the maximum number of ECM-containable blocks in the problem.

Step 3: Having chosen L, determine the number of blocks (U) to be ECM-contained:

(a) Determine the upper bound for U satisfying W(U,L) < WMAX. Graphical determination using the domain in Fig. 3.4 bounded by the lines WMAX and L and by the bandwidth curves B<M provides the quickest solution.

(b) Determine the minimum number of I/O passes (P)

P = (M-1) / (L*U) + 1

required to perform the inner iterations for each group during each outer iteration.

(c) Minimize U subject to P (just as in the example at the start of this section), i.e. calculate

U = (M-1) / (L*P) + 1 .

Step 4: Calculate ECMCC, the ECM container size for the CIIS

ECMCC = ECMISC + W(U,L)*I*J.

The above procedure minimizes I/O operations and memory requirements subject to the fixed values of parameters MINBSZ, M and ECMMAX. In analyzing a particular job, one should be cognizant of the fact that there is a certain level of performance uncertainty largely attributed to the presence of overlapped I/O and CPU operations and to the subjectiveness of the optimal value for the MINBSZ parameter. The degree of overlap (concurrency) achieved relative to the potential overlap attainable is influenced by the resident job mix at execution time as well as the parameters U and L. Depending on the charging algorithm employed, it may be cheaper at certain host installations to arbitrarily reduce region size at the expense of I/O or vice versa to obtain reduced overall job cost or improved turnaround time.

3.11 Criticality Search Input and Edits

The primary means for specifying criticality search data is via the A.NIP3 type 21-26 cards. The card-by-card description of A.NIP3 is found in APPENDIX B.4.

The general form of the search equations is

P(x) = P(0) + x * M

where P is the quantity being varied. The user must specify the following data:

1. the parametric modifiers M of the search quantity P
2. bounds for and two initial estimates of the search parameter x
3. the desired search k-effective, k_d;
4. the search k-effective convergence criterion (EPSRCH);
5. the maximum number of search passes permitted.

The alternative to criticality search data specification via A.NIP3 is to supply the CCCC standard interface file SEARCH. The SEARCH file description provided in APPENDIX C indicates the subset of SEARCH options implemented at ANL and the corresponding ANL modifications to SEARCH.

The code block GNIP4C reads A.NIP3 and writes a SEARCH file when the appropriate type 21-26 cards are present.

3.11.1 Parametric Modifiers M - A.NIP3 23-26 Cards

The desired search option is indicated by the presence of one of the four mutually exclusive A.NIP3 type 23-26 cards. DIF3D currently permits only a nuclide concentration search via the type 23 card of A.NIP3.

The nuclide concentration search operates on subzone volume fractions, modifying the net atom densities in each zone (composition) to which the modifier subzone is assigned. Modifier subzones and the zones they modify are both specified on the type 23 card of A.NIP3.

3.11.2 Search Parameter Estimates x - A.NIP3 22 Card

Two initial estimates for the criticality search parameter and upper and lower bounds for the search parameter during the course of the search are specified on the type 22 card of A.NIP3. The search problem should be formulated such that the magnitude of the search parameter estimate satisfies ($.1<x<1.0$) for best performance of the parabolic interpolation option of the search procedure. The A.NIP3 type 22 card is optional.

3.11.3 Search Pass Control Parameters - A.NIP3 21 Card

Search passes are normally terminated by one of four conditions:

1. search convergence;
2. the maximum number of search passes reached;
3. computing time limit detected;
4. the search parameter out of range.

The user specifies the desired k-effective, the relative k-effective error bound (EPSRCH) and the maximum number of search passes on the type 21 card of A.NIP3. Specification of the search parameter range restrictions is discussed in the previous section.

From an efficiency standpoint it is recommended that the neutronics calculation k-effective convergence criterion (ε_k) be no more than an order of magnitude tighter than EPSRCH during the search passes. Upon search convergence the flux can be more tightly converged via an appropriate restart of the neutronics problem.

3.11.4 Search Restarts - A.NIP3 21 and 22 Cards

In the event of abnormal termination, or if tighter k-effective convergence is desired, the search pass loop may be efficiently restarted by supplying the appropriately saved SEARCH, RTFLUX and DIF3D files and by specifying them under "BLOCK=OLD" in the BCD input data. Data supplied on the type 21 and 22 cards of A.NIP3 will override corresponding data items on the existing SEARCH file.

3.11.5 Search Edits - A.NIP3 21 Card

An edit of a newly created or a previously existing SEARCH file may be obtained from GNIP4C via a sentinel on the type 21 card of A.NIP3. Sentinels for editing the search parameter data and the search quantity at each search pass are also provided on the type 21 card of A.NIP3.

A sentinel provided on the type 04 card of A.DIF3D permits user control of the frequency of the DIF3D neutronics edits. The latter edits are usually deferred until search convergence.

3.12 Running DIF3D

3.12.1 Input and Output Interface Datasets

The BCD and binary input and output files potentially encountered during the execution of DIF3D are tabulated in Table 3.4. User input and output options are such that only a problem dependent subset of these files are required. The next several subsections address details pertinent to the execution of DIF3D on specific classes of host system environments. Much of this discussion is based on DIF3D implementation experience gained on computers which are representative of each environment class.

3.12.2 Sample Input

Figure 3.5 illustrates a job input deck for Sample Problem 1 in the National Energy Software Center (NESC) package (see Section 5.3). The microscopic cross section file ISOTXS is supplied in BCD card image form via the A.ISO file. In typical production applications the ISOTXS binary interface file is usually specified under BLOCK=OLD since it is generated by appropriate cross section processing codes. The remaining interface file data is specified using free format input.

TABLE 3.4. DIF3D Interface Files (CCCC and code-dependent)

BCD	Binary	Mode[a]	Contents
	GEODST[b]	I/S	Model Geometry
	NDXSRF	I/S	Composition definition
A.NIP3	ZNATDN	I	(Sub) Zone atom densities
	FIXSRC	I	Distributed inhomogeneous source
	SEARCH	I/R	Criticality search specifications
A.ISO	ISOTXS	I	Microscopic cross sections
	XS.ISO	I	Converted to ISOTXS by CSE010
A.HMG4C		I	HMG4C control parameters
	COMPXS[b]	I/S	Macroscopic cross sections[c]
A.DIF3D	DIF3D[b]	I/R	DIF3D control parameters
A.LASIP3		I	LASIP3 input processor data
	RTFLUX[d]	O/R	Real flux
	ATFLUX[d]	O/R	Adjoint flux
	NHFLUX[e]	O/R	Nodal real solution vectors
	NAFLUX[e]	O/R	Nodal adjoint solution vectors
	RZFLUX	O	Real zone averaged flux
	PWDINT	O	Power density
	PKEDIT	O	Peak power and flux by mesh cell
	D3EDIT	O	DIF3D integral edits

[a]File usage (I=Input, O=Output, R=Restart, S=Modified by SRCH4C)
[b]Binary input files ultimately required by DIF3D.
[c]Can be created from ISOTXS, NDXSRF and ZNATDN by HMG4C.
[d]Binary output files required by DIF3D (RTFLUX and/or ATFLUX).
[e]Binary output files required by DIF3D nodal option (NHFLUX and/or NAFLUX).

```
//SAMPLE1  JOB REGION=1200K,TIME=3,CLASS=W
//*MAIN ORG=PRO,LINES=10
// EXEC ARCSP021,RTFLUX='C116.B20245.SAMPLE.RTFLUX',
//                RTCYL=1,RTDSP=(NEW,CATLG)
//SYSIN DD *
BLOCK=STP021
NOSORT=A.ISO
      <A.ISO dataset is listed in Fig. 5.1>
UNFORM=A.NIP3
      <A.NIP3 dataset is listed in Fig. 5.1>
UNFORM=A.DIF3D
      <A.DIF3D dataset is listed in Fig. 5.1>
```

Fig. 3.5. ANL DIF3D Input Skeleton for Sample Problem 1

When the required binary files already exist (possibly created via an alternative CCCC interface file input processor), the minimal input data illustrated in Fig. 3.6 is sufficient to run DIF3D. At Argonne it is occasionally convenient to employ LASIP3,[37] a generalized BCD input processor code block for CCCC standard interface files. Figure 3.7 illustrates a skeleton of the input data required to execute LASIP3. The optional FPRINT data set supplied in the A.LASIP3 input specifies selective edits of the CCCC interface file data.

3.12.3 IBM Considerations - ARCSP021 Symbolic Parameters

Several key Job Control parameters including Job REGION size and Job TIME limit must be specified by the user. Table 3.5 contains the formula for computing the Job REGION size which must include space for the FCM and ECM containers in addition to the space required for the DIF3D program and its I/O buffers. CPU time requirements depend upon the problem size and type, and the data management option employed. At Argonne no limit is placed on the I/O activity in a job; the EXCP's component of the current charging algorithm assesses the use of I/O resources. Therefore, the EXCP charge is influenced directly by the active DIF3D management option and typically accounts for 30 to 40% of the job cost in large problems.

CPU times for the finite-difference option in DIF3D are roughly linear with the number of flux work units (MFWU) defined by:

$$\text{MFWU} = 10^{6} \cdot \text{NCELLS} \cdot \text{N} \cdot \sum_{g} m_g$$

where NCELLS is the number of space mesh cells, N is the number of outer iterations and m_g is the number of inner iterations in group g. The m_g are constant throughout the problem and typically range between 8 to 25 inners per outer, m_g increases monotonically as the spectral radius increases. The upper end of this range is typically achieved in problems having very fine mesh width specifications. Typical ranges for the number of outer iterations vary between 15 to 25 iterations to achieve the default convergence criteria. The higher values in this range are achieved as the dominance ratio (the ratio of the fundamental eigenvalue to the first harmonic) increases towards its limiting value of unity.

Based upon statistics gathered from a variety of DIF3D jobs run on the IBM 370/195 computers, typical computation rates between 6 and 12 MFWU per minute are standard. Problems with large numbers of mesh cells in the first coordinate ("X") dimension achieve even higher values. For example, the 1 cm mesh (170 × 170) 2D IAEA benchmark problem (see general description in Section 5.3.2) achieves 17 MFWU. This corresponds to 3.9 megaflops (millions of floating point operations per second) when the 13 floating point operations (add or multiplies) per FWU in two-dimensional problems are considered. Lower computation rates are encountered in triangular geometry problems due to additional computational overhead. The ratio of EXCP to CPU charges in triangular geometry problems is also increased due to the extra background mesh cells which are carried along for coding convenience but are not within the solution domain.

```
BLOCK=OLD
DATASET=GEODST
DATASET=ISOTXS
DATASET=NDXSRF
DATASET=ZNATDN
BLOCK=STP021
UNFORM=A.DIF3D
.
.
.
/*
```

Fig. 3.6. Minimal Input Data Example

```
BLOCK=OLD
DATASET=NDXSRF
DATASET=ZNATDN
BLOCK=STP021
UNFORM=A.DIF3D
   .
   .
   .
NOSORT=A.LASIP3
        5000    / (6X,4I6) BPOINTER container size (see Section 3.13)
OV FPRINT
 1D 4000        / Process four files with the print
 2D GEODST 0000 / Print all GEODST record types
 2D ISOTXS 0032 / Print three record types and two isotopes
 3D 1  4 5      / ISOTXS record types to be printed
 4D 1  4        / ISOTXS isotopes to be printed
 2D NDXSRF 0000 / Print all NDXSRF record types
 2D ZNATDN 0000 / Print all ZNATDN record types

OV GEODST
   .
   .
   .
OV ISOTXS
   .
   .
   .
STOP
/*
```

Fig. 3.7. LASIP-3 Input Skeleton

TABLE 3.5. Job Region Size and Dataset Space Estimation for ARCSP021

Parameters

NCELLS = Number of mesh cells in the problem
NDIM = Number of problem dimensions (1, 2 or 3)
NGROUP = Number of energy groups
NGUP = First group with nonzero upscatter source
S = 2*NDIM-0, number of orthogonal geometry surfaces
= 2*NDIM-1, number of triangular geometry surfaces
ECM = ECM or FCM container size[a]
PROGSIZE = 325K bytes, the storage required for DIF3D program and I/O buffers

REGION = (ECM+FCM)/128 + PROGSIZE = JOB CARD Region Size

Data Set Space Allocation Estimation

ARCSP021 Symbolic Parameters[b]	Dataset Name	FTXXF001		Storage Estimate Cylinders
FLXCYL(1)	group independent data	46-49,51,55,56	=	NCELLS*8/CYLSIZ[c]
ZONCYL(1)	ZONMAP	52	=	FLXCYL/2
RTCYL(5)	RTFLUX	30	=	FLXCYL*NGROUP
ATCYL(5)	ATFLUX	31		
PSICYL(5)	PSINEW	41		
PSICYL	PSIOLD	42		
PSICYL	FSRC	54		
PSUCYL(3)	NGUP	43	=	FLXCYL*(NGROUP+1-NGUP)
FDCCYL(20)	FDCOEF	45	=	PSICYL*(NDIM+1)
DMY1CYL(21)	&&DUMMY1	DUMMY1	=	FDCCYL+ZONCYL
DMY2CYL	&&DUMMY2	DUMMY2	=	PSICYL+FLXCYL*2
DMY2CYL(7)	&&DUMMY3	DUMMY3		
DMY2CYL	&&DUMMY4	DUMMY4		
DMY5CYL(5)	&&DUMMY5	DUMMY5	=	PSUCYL+FLXCYL
SRFCYL(12)	SCR001 SCR002	66,67	=	2*NCELLS*(S+1)/CYLSIZ

[a]Refer to Table 3.2.

[b]Symbolic parameter defaults are enclosed in parenthesis.

[c]CYLSIZ is dependent on device type and block size. When the BLKSIZE=6136, CYLSIZ=12280*19 on a 3330 disk (CYLSIZ=18416*30 on a 3350 disk).

Many files are accessed during the course of a DIF3D calculation and each of them requires a Data Definition (DD) card to describe the file characteristics including size allocations, disposition, volume identification, DCB information and the dataset name. To simplify the input deck for users of the ANL IBM computers a cataloged procedure (ARCSP021) was written (see listing in Appendix A). Symbolic procedure parameters in ARCSP021 permit convenient user specification of key parameters for various DD cards without recoding the entire DD statement. Comments within the ARCSP021 procedure tabulate the default values and usage of the symbolic parameters and the logical unit numbers (FTnnF001) to which they apply. Several symbolic parameters deserve special attention and are described in the following paragraphs.

The default value (RECFM=U) of the symbolic parameter MODEDCB designates thirteen files as random access I/O files to the I/O package (SIO) employed by DIF3D. An attempt to minimize disk head contention is made by suballocating these files in a particular ordering among the five available scratch disk volumes at ANL. The user must override the default space allocations for these files when the space estimation formulas in Table 3.5 indicate the default values are insufficient. The formulas provide allocation estimates for the thirteen individual files, for RTFLUX and ATFLUX files, and for the five dummy datasets on which the thirteen scratch files are suballocated. When estimating the cylinder sizes for the dummy datasets all fractions must be rounded to the next highest integral number of cylinders. Appropriate cylinder sizes are edited for all ARCSP021 parameters immediately before the data management summary page.

The parameters UNITSCR=SASCR and UNITS=BATCHDSK denote the system scratch disk volumes and the pool of disk volumes on which datasets can be cataloged, respectively. The latter designation is given to files which are deemed likely to be cataloged by a user.

All files but the thirteen random access files are given block size parameters appropriate to their anticipated I/O activity. When explicitly overriding JCL for any file care must be exercised to specify block sizes appropriate to the output device type so as to avoid inefficient use of storage space.

Insufficient disk storage for extremely large jobs require users to assign the largest scratch file FT45F001 to a 6250 BPI scratch tape. In this event the entire DD card is overridden with the following alternate specification:

```
//FT45F001 DD UNIT=READ6250,SUBALLOC=,
//      DCB=(RECFM=VBS,LRECL=X,BLKSIZE=12280,DEN=4)
```

If the job using a scratch tape has the possibility of running on OS/MVT (i.e. the IBM/195), then some additional JCL is needed to prevent the operator from issuing a tape save request which assigns the tape to the user's account. The following two steps are recommended:

1. Add the following JCL as the first step of the job

```
//STEP1    EXEC PGM=IEFBR14
//$$NOSAVE DD   VOL=SER=,UNIT=READ6250,DISP=(NEW,PASS),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=12280,DEN=4)
```

2. then override the FT45F001 card:

```
//FT45F001 DD UNIT=READ6250,SUBALLOC=,
// VOL=REF=*.STEP1.$$NOSAVE,DISP=(NEW,DELETE),
// DCB=(RECFM=VBS,LRECL=X,BLKSIZE=12280,DEN=4)
```

3.12.4 CDC 7600 Considerations

Figures 3.8 and 3.9 illustrate the structure of a typical job to be executed on the CDC 7600 at Lawrence Berkeley Laboratory (LBL) and at Brookhaven National Laboratory (BNL), respectively. The problem to be solved is identical to that shown in Figure 3.5. As in the latter example for IBM systems, the assumption is made that an absolute overlay module already exists and in this example is merely "STAGEd in" from a magnetic tape library.

When the DIF3D absolute overlay module is created, minimum field length requirements for all subsequent executions of this module can be easily obtained by scanning the loader map for the maximum SCM and LCM field lengths. These field lengths are dynamically requested prior to invoking DIF3D using either the SFL card at LBL or the RFL card on "off the shelf" CDC systems such as the system at BNL. A nominal field length sufficient to perform the staging is specified on the JOB card in these examples.

Additional SCM or LCM field length required for BPOINTER containers subsequently used in DIF3D is dynamically allocated and deallocated appropriately during the execution. In fact, the user must not preallocate space for the BPOINTER containers since DIF3D only uses space dynamically allocated by DIF3D. Error messages result when insufficient field length is available for dynamic allocation. Consequently, the user never needs to compute the SCM and LCM field lengths associated with the BPOINTER container sizes.

On standard CDC installations such as the one at Brookhaven National Laboratory, less SCM space is demanded by the I/O buffers. About 70,000 octal SCM words are required, thereby permitting a substantial increase in the FCM container size.

Upper bounds for computing units (CU's) at LBL or Central Processor (CP) seconds at BNL are also required on the JOB card. Estimates of CP seconds for the CDC 7600 are from 10 t 25% less than the corresponding estimates for the IBM 370/195 (see Section 3.12.3). The CU's quantity at LBL is defined as

```
CU=3*CP+.5*BLD+ITO.
```

The BLD quantity is discussed below. The interference to others (ITO) quantity measures the efficiency of the utilization of system resources acquired by a job. Figuring heavily in the ITO computation is the LCM size and the frequency of I/O requests.

The relatively simple Job Control Language on CDC systems simplifies the user's dealings with the many binary files required by DIF3D. Two I/O related considerations, however, are pertinent to execution at LBL.

A significant fraction of the cost of executing jobs requiring large amounts of disk to ECM data transfers is based on the number of buffer loads (BLD). Therefore it is desirable to reduce the number of BLD's by increasing the size of LCM system buffers for the large files when they are not core-contained. This is accomplished via the control card

```
FBSIZE,filename=m.
```

```
LBLJOB,7,600,10000.xxxxxx,username
GBSIZE,20.
GETTAPE,DIF3D/*,nnnnn.
GBSIZE,5.
FBSIZE,DIF3D=100.
SFL,120000,1.
DIF3D,LC=77777.
FILES.
7-8-9 END-OF-RECORD CARD
BLOCK=STP021
NOSORT=A.ISO

<See A.ISO DATASET specified in Fig. 5.1>

UNFORM=A.NIP3

<See A.NIP3 DATASET specified in Fig. 5.1>

UNFORM=A.DIF3D

<See A.DIF3D DATASET specified in Fig. 5.1>

6-7-8-9 END-OF-INFORMATION CARD
```

Fig. 3.8. Structure of Job Deck for CDC 7600 at LBL

```
BNLJOB,T400,CM20000.
STAGE,DIF3DUB,E,PE,VSN=KXXXX.
REWIND,DIF3DUB.
COPYBF,DIF3DUB,DIF3D.
RETURN,DIF3DUB.
RFL,70000,L=1.
DIF3D.
7-8-9 END OF RECORD CARD
BLOCK=STP021

<See identical input data record in Fig. 3.8.>

6-7-8-9 END-OF-INFORMATION CARD
```

Fig. 3.9. Structure of Job Deck for CDC 7600 at BNL

where filename is the appropriate file name and m is the buffer size in units of 1000 words. m=100 is recommended for large files. In all problems it is recommended that a global buffer size value be changed to 20 by the control card

```
GBSIZE=20.
```

as in the example in Figure 3.8, thereby attempting to reduce the BLD costs for all files.

The control card, FILES, provides detailed information concerning the BLD's and sectors required by each file in a job, and is useful for determining the distribution of I/O costs by file name. If used it should be inserted at the end of the control card record.

The control card

```
DISKHOG,n.
```

is required to override the default limit of 4000 sectors when problems which use more than 4000 disk sectors must be executed. The DISKHOG card should be inserted after the JOB card.

An estimate of the number of sectors, n, required by a given job can be obtained from the following formula

$$n = 1.1 * NCELLS * 2 + NGROUP * (5+NDIM)$$

where the variables are defined in Table 3.2. The estimate for n is made with the assumption that the major scratch files on logical units (41, 42, 45, 48, 49 and 53) are on disk.

3.12.5 Multiple Problems and Restarts - RTFLUX and DIF3D

Practical economic reasons necessitate the inclusion of a restart capability in DIF3D. This feature primarily permits the resumption of the outer iteration process from the point of termination by employing the RTFLUX (ATFLUX) file saved when the previous job terminated (gracefully). It is also advantageous to supply the optimum overrelaxation factors during restarts because they account for 5 to 10% of the cost in most calculations without restarts. The simplest way to supply these factors is to save the DIF3D restart dataset named DIF3D. It contains the DIF3D control parameters, the most recently updated k-effective and dominance ratio estimates, and the optimum overrelaxation factors.

For certain classes of problems it is economical to retain a fixed set of optimum overrelaxation factors for the entire set of similar jobs. These factors are always identical for real and adjoint calculations of a given problem configuration. Control rod worth studies as well as many criticality search problems frequently yield practically identical convergence rates with the initially computed set of optimum overrelaxation factors.

From time to time users attempt to reduce computing times by starting off with an initial flux guess which is the converged solution of a related

problem configuration. This is probably most effective in near-critical fixed source problems where the magnitude of the flux is an important factor. Problems requiring thermal iterations are likely to benefit from this practice also. However, situations have been encountered where the use of initial flux guesses require additional outer iterations to satisfy the same convergence criteria as that attained by a similar calculation with an initial flat flux guess.

It is sometimes convenient to stack similar model cases in a single job step by employing successive sets of BLOCK=STP021 data blocks. Unless explicitly REMOVEd by an appropriately placed REMOVE=filename input command, previously created, binary and BCD files remain in existence. Consequently, the binary interface file ultimately to be changed must be explicitly removed so that the modified file can be created. Typical candidates here are the CCCC interface files GEODST, COMPXS, NDXSRF and/or ZNATDN.

3.13 LASIP3 CCCC Standard Interface File Processor

LASIP3[37] will permit the specification and editting of all CCCC interface files. In the Argonne implementation of LASIP3, two additional card-images must immediately precede the normal LASIP3 input data specified in Ref. 37. The first of these card-images must be the NOSORT=A.LASIP3 card which signals the start of LASIP3 input. The second contains BPOINTER control information and a data item LASTCL that indicates the number of columns (default=72) to be processed by the LASIP3 free-field input processor. The card has the format (6X, 4I6) and contains the four data items: MAXSIZ, MAXBLK, IPRINT and LASTCL. MAXSIZ is the FCM container size in long (REAL*8) words. MAXBLK is unused. IPRINT is the BPOINTER debugging sentinel and has input options identical to those described on the A.DIF3D type 02 card. A MAXSIZ value of 5000 to 10000 is usually quite adequate for most applications. However, a conservative approach is simply to supply a container size bounded by the sum of the FCM and ECM sizes on specified in A.DIF3D. Figure 3.7 contains an example of data set A.LASIP3.

3.14 Definitions of Output Integral Quantities

As noted in Section 3.9.4, DIF3D provides optional edits of commonly expected flux integral quantities. Five sentinels (items 5-9) on the type 04 card of dataset A.DIF3D provide the user with the ability to select the desired subset of edits. The sentinels for items 5, 6 and 7 are multidigit numbers which permit edits by region and/or group, and by mesh cell and/or group (see Appendix B.1).

The definition of the various integrals for each of the five major edit options are tabulated separately and in the order of their appearance in the individual edits. A preliminary subsection is devoted to establishing the definitions and notation for the integral forms used in the tabulation. An explanation of the iteration history page is also included.

3.14.1 Iteration History Quantities

In multidimensional geometries the iteration history page begins with a tabulation of the group-dependent inner iteration optimum overrelaxation factors w_g together with m_g the corresponding fixed number of inner iterations per outer iteration. These factors are absent in the one-dimensional case because the resulting tridiagonal inner iteration matrix is solved directly.

Following the optimum factor edit, a one-line summary of key parameters for each outer iteration is printed. The first three items are outer iteration convergence criteria:

1) the relative pointwise fission source error,

$$\varepsilon_{\lambda}^{(n)} = \frac{\bar{\lambda}^{(n)} - \underline{\lambda}^{(n)}}{2}, \tag{3.7}$$

monitors the pointwise eigenvector convergence;

2) the relative fission source sum error,

$$\varepsilon_{\psi}^{(n)} = \frac{\| \underline{\psi}^{(n)} - \underline{\psi}^{(n-1)} \|_2}{\left(\underline{\psi}^{(n)}, \underline{\psi}^{(n-1)} \right)^{1/2}}, \tag{3.8}$$

monitors the average eigenvector convergence;

3) the eigenvalue change,

$$\varepsilon_{k}^{(n)} = k_{eff}^{(n)} - k_{eff}^{(n-1)}, \tag{3.9}$$

is a measure of the eigenvalue convergence.

Next in appearance are three items pertinent to the Chebyshev acceleration of the outer (power) iterations:

1) the order p of the Chebyshev polynomial in the current extrapolation cycle;

2) $\hat{\sigma}$, the dominance ratio estimate for $\bar{\sigma}$ to be used in Eq. (2.61);

3) $\hat{\sigma}'$ is the most recent update for the dominance ratio estimate (see Eq. 2.84).

When the Chebyshev acceleration is not applied, p and $\hat{\sigma}$ will be zero.

The last item on each history line is $k_{eff}^{(n)}$ which is computed during outer iteration n (see Eq. 2.92), except during external source problems in which case $k_{eff}^{(n)} \equiv \mu$ is constant and is followed by the (unnormalized) total fission source integral for the reactor. In fixed source problems the dominance ratio estimates are replaced by the spectral radius estimates of the outer iteration matrix.

Upon termination of the outer iterations one of three messages appear:

1) outer iterations converged;

2) maximum number of outer iteration achieved;

3) time limit exceeded.

This message is followed by the most recent eigenvalue estimate and a summary edit of the parameters needed for a subsequent restart of the terminating DIF3D job.

In most problems the relative pointwise fission source error in Eq. (3.6) is the quantity most frequently monitored by users to indicate satisfactory convergence. The eigenvalue change (Eq. (3.8)), an integral parameter, usually is several orders of magnitude less than the pointwise monitor.

3.14.2 Preliminary Definition of Integral Forms

The output tabulations include flux distributions by mesh cell and integrals of the flux including power distribution and neutron balances by region and/or group. Note, that throughout this section we frequently use the full subscript ijk when only ij or i are required. In such cases the redundant subscripts may be assumed to be unity. Note also that the * superscript is left off adjoint fluxes.

All tabulations are based on weighted integrals of the flux as a function of three spatial variables and one energy variable with the integrals extending over the domain of the reactor.

Region-dependent extrapolated half heights $\bar{H}_{rn}$, n=1,N may be optionally specified for the N(=1 or 2) transverse directions in one- or two-dimensional problems. The $\bar{H}_{rn}$ generate the cosine flux shape $W_{rn}(\xi_n)$.

$$W_{rn}(\xi_n) \equiv \begin{cases} \cos \dfrac{\pi \xi_n}{2\bar{H}_{rn}} & n = 1 \text{ or } 2 \\ 1 & n = 0 \end{cases} \tag{3.10}$$

in transverse direction ξ_n. The notation is generalized to include n=0, the case when $\bar{H}_{rn}$ is unspecified, so that the following two equations summarize the flux shapes that may be assumed in DIF3D:

1. X, XY, XYZ or triangular (T or TZ) geometries:

$$\phi(x,y,z) = \prod_{n=0}^{N} W_{rn}(\xi_n) \cdot \begin{cases} \phi(x) & N = 0, 1 \text{ or } 2 : X \\ \phi(x,y) & N = 0 \text{ or } 1 : XY \text{ or } T \\ \phi(x,y,z) & N = 0 : XYZ \text{ or } TZ \end{cases} \tag{3.11}$$

2. R, RZ, θR, θRZ geometries:

$$\phi(\theta,r,z) = \prod_{n=0}^{N} W_{rn}(\xi_n) \cdot \begin{cases} \phi(r) & N = 0 \text{ or } 1 : R \\ \phi(r,z) & N = 0 \quad : RZ \\ \phi(\theta,r) & N = 0 \text{ or } 1 : \theta R \\ \phi(\theta,r,z) & N = 0 \quad : \theta RZ \end{cases} \tag{3.12}$$

where the product symbol is defined by

$$\prod_{n=0}^{N} t_n = t_0 \cdot t_1 \cdot t_2 \cdot \ldots \cdot t_n .$$

Consider any macroscopic cross section $\Sigma_r^{x,g}$ in region r (having unextrapolated half-height H_{rn}). Using XY geometry as an example a typical integral edit might involve the numerical approximation to the following integral

$$I_r^g = W_r \iint_{x,y \in r} dxdy \; \Sigma_r^{x,g} \phi^g(x,y)$$

$$\tilde{=} \; W_r \Sigma_r^{x,g} \sum_{i,j \in r} \phi_{ij}^g(x,y) V_{ij} \tag{3.13}$$

where the V_{ij} are defined in Table 2.2 and the flux integration weight factor is defined by

$$W_r = \begin{cases} 1 & \text{for } N = 0 \\ \prod_{n=1}^{N} \int_{-H_{rn}}^{H_{rn}} d\xi_n W_{rn}(\xi_n) & \text{for } N = 1 \text{ or } 2 \end{cases} \tag{3.14}$$

In this case

$$W_r = \frac{4H_{r1}}{\pi} \sin\left(\frac{\pi \bar{H}_{r1}}{2H_{r1}}\right). \tag{3.15}$$

A second weighting factor, the volume integration weight factor

$$W_r^v = \begin{cases} 1 & N = 0 \\ \dfrac{N}{\prod_{n=1} 2H_{rn}} & N = 1 \text{ or } 2 \end{cases} \tag{3.16}$$

is required to compute region volumes

$$V_r = W_r^v \sum_{ijk \epsilon r} V_{ijk} \tag{3.17}$$

and the total reactor volume

$$V_T = \sum_r V_r. \tag{3.18}$$

In real homogeneous problems the flux is normalized to the user-specified power level, P_o, i.e.

$$\phi_{ijk}^g = N^P \phi_{ijk}^{g(\text{computed})} \tag{3.19}$$

The normalization factor N^P is calculated the following way

$$N^P = \begin{cases} P_o/P_u & \text{for real homogeneous problems} \\ 1 & \text{for adjoint homogeneous and fixed source problems} \end{cases} \tag{3.20}$$

where

$$P_u = \sum_{g=1}^{G} \sum_{r=1}^{R} W_r \psi_r^g \tag{3.21}$$

$$\psi_r^g = \sum_{ijk \epsilon r} PC_r^g V_{ijk} \phi_{ijk}^{g(\text{computed})}. \tag{3.22}$$

PC_r^g is the power conversion factor, see the COMPXS description in Appendix D.1.

DIF3D permits the user to specify arbitrary collections of regions (called areas) over which the various output integrals are to be performed. A typical integral over area a is defined in terms of region integrals, i.e.

$$I_a^g = \sum_{r \in a} I_r^g. \tag{3.23}$$

If areas exist, they will be editted whenever region edits are requested. The region to area assignments are recorded in the 2D record of the LABELS file (see Appendix D.3).

Improved accuracy may be obtained for peak flux and power edits based on pointwise flux or power distributions if the average flux distribution $\phi_{ijk}^{g,m}$ on the m = 1,2,...,M surfaces of each mesh cell are computed in addition to the cell-averaged flux. (The surface index assignments follow the conventions of Section 2.1.2 where m = 1 for -x, m = 2 for +x,..., m = 6 for +z.) M = 2N in orthogonal geometry where N = 1,2 or 3 denotes the number of coordinate directions in the problem. In triangular geometry M = 2N-1 because only a single second-dimension surface assignment is required to index the alternating pattern of upper and lower triangle surfaces.

Equation (2.18) in the finite-difference coefficients derivation provides an interpolation formula that yields surface-averaged fluxes with an $O(h^2)$ accuracy consistent with that of the cell-averaged fluxes, i.e. for m = 2

$$\phi_{ijk}^{g2} = \frac{\frac{D_{ijk}^g}{\Delta x_i}}{\frac{D_{ijk}^g}{\Delta x_i} + \frac{D_{i+1jk}^g}{\Delta x_{i+1}}} \phi_{ijk}^g + \frac{\frac{D_{i+1jk}^g}{\Delta x_{i+1}}}{\frac{D_{ijk}^g}{\Delta x_i} + \frac{D_{i+1jk}^g}{\Delta x_{i+1}}} \phi_{i+1jk}^g \tag{3.24}$$

Consistent with this notation the cell-averaged flux is assigned to index M+1, i.e.,

$$\phi_{ijk}^{gM+1} \equiv \phi_{ijk}^g. \tag{3.25}$$

We can now display the calculations made in the five edit categories.

3.14.3 Region and Mesh Cell Flux Integrals

1. Neutron flux by mesh cell and group (RTFLUX or ATFLUX)

$$\phi_{ijk}^g = N^p \varphi_{ijk}^{g(\text{computed})}$$

2. Group-integrated neutron flux by mesh cell

$$\phi_{ijk} = \sum_{g=1}^{G} \phi_{ijk}^{g}$$

3. Region and/or group and area flux integrals

a. Total flux (neutron-cm/sec)

$$\phi_r = \sum_{g=1}^{G} \phi_r^g, \quad \phi_T = \sum_r \phi_r,$$

$$I_a = \sum_{r \in a} \phi_r$$

where ϕ_r^g is defined using Eq. (3.13) with $\Sigma_r^{x,g} \equiv 1$.

b. Peak group-integrated mesh cell flux (neutron/cm^2-sec)

$$\hat{\phi}_r = \max_{1 \le m \le M+1} \left| \phi_{ijk}^m \right|, \quad \hat{\phi}_T = \max_r \hat{\phi}_r,$$

$$\hat{\phi}_a = \max_{r \in a} \hat{\phi}_r$$

c. Total fast flux (neutron-cm/sec)

$$\phi_r^f = \sum_{g=1}^{g'} \phi_r^g - \alpha \phi_r^{g'}, \quad \phi_T^f = \sum_r \phi_r^f,$$

$$\phi_a^f = \sum_{r \in a} \phi_r^f$$

where

$$\alpha = 1 - \frac{\ln(E_{100}/E_{max}^{g'})}{\ln(E_{min}^{g'}/E_{max}^{g'})}$$

E_{100} = 100 keV, the fast flux energy threshold

g' = energy group in which $E_{min}^{g'} < E_{100} < E_{max}^{g'}$

E_{max}^g and E_{min}^g are the maximum and minimum energy bounds for group g

d. Peak mesh cell fast flux (neutrons/cm^2-sec)

$$\hat{\phi}^f_r = \max_{1\le m\le M+1} \left|\phi^{f,m}_{ijk}\right|, \quad \hat{\phi}^f_T = \max_r \left|\hat{\phi}^f_r\right|,$$

$$\hat{\phi}^f_a = \max_{r\in a} \hat{\phi}^f_r$$

where

$$\phi^{f,m}_{ijk} = \sum_{g=1}^{g'} \phi^{g,m}_{ijk} - \alpha\phi^{g',m}_{ijk}$$

e. Total flux by region and group (neutron-cm/sec)

$$\phi^g_r = W_r \sum_{ijk\in r} \phi^g_{ijk} V_{ijk}, \quad \phi^g_T = \sum_r \phi^g_r$$

$$\phi^g_a = \sum_{r\in a} \phi^g_r$$

3.14.4 Region-Averaged Flux Integrals

Average total flux by region (neutron/cm^2-sec)

$$\bar{\phi}_r = \sum_{g=1}^{G} \phi^g_r/V_r, \quad \bar{\phi}_T = \phi_T/V_T$$

$$\bar{\phi}^g = \phi^g_r/V_r, \quad \bar{\phi}^g_T = \phi^g_T/V_T$$

3.14.5 Zone-Averaged Flux Integrals (RZFLUX)

Average total flux by zone (neutron/cm^2-sec)

$$\bar{\phi}_c = \sum_{r\in c} \sum_{g=1}^{G} \phi^g_r /V_c, \quad \bar{\phi}^g_T = \phi_T/V_T$$

$$\bar{\phi}^g_c = \sum_{r\in c} \phi^g_r/V_c, \quad \bar{\phi}^g_T = \phi^g_T/V_T$$

where

$$V_c = \sum_{r \epsilon c} V_r$$

3.14.6 Region and Mesh Cell Power Density Integrals (PWDINT)

1. Power density by mesh cell (PWDINT interface file):

$$P_{ijk} = \sum_{g=1}^{G} PC^g_{ijk} \phi^g_{ijk}$$

2. Region, region-integrated and area tabulation:

   a. Flux integration weight factor W_r (see Eq. (3.14))

   b. Total power (watts)

$$P_r = \sum_{g=1}^{G} PC^g_r \phi^g_r$$

$$P_T = \sum_{r} P_r$$

$$P_a = \sum_{r \epsilon a} P_r$$

   c. Average power density (watts/cc)

$$\bar{P}_r = P_r / V_r$$

$$\bar{P}_T = \sum_{r} P_r / \sum_{r} V_r$$

$$\bar{P}_a = \sum_{r \epsilon a} P_r \sum_{r \epsilon a} V_r$$

   d. Peak power density

$$\hat{P}_r = \max_{\substack{ijk \epsilon r \\ 1 \le m \le M+1}} \left| P^m_{ijk} \right|$$

$$\hat{P}_T = \max_r \left|\hat{P}_r\right|$$

$$\hat{P}_a = \max_{r\epsilon a} \left|\hat{P}_r\right|$$

e. Peak-to-average power density:

$$P_r^A = \hat{P}_r/\bar{P}_r$$

$$P_T^A = \hat{P}_T/\bar{P}_T$$

$$P_a^A = \hat{P}_a/\bar{P}_a$$

f. Mesh cell indices $(i,j,k)_p$ associated with peak power density of type p where $p = \hat{P}_r$, $\hat{P}_T$ or $\hat{P}_a$.

g. Power density (three-dimensional problems only) in the axial column of mesh cells in area a that includes the mesh cell location $(i,j,k)\hat{P}_T$

$$P_a^z = \sum_{g=1}^{G} \sum_{r\epsilon a} \sum_{\substack{ijk\epsilon r \\ ij=(i,j)\hat{P}_T}} PC_{ijk}^g \phi_{ijk}^g V_{ijk} \Bigg/ \sum_{r\epsilon a} \sum_{\substack{ijk\epsilon r \\ ij=(i,j)\hat{P}_T}} V_{ijk}$$

h. Peak-to-average power density in the axial column described for the preceding item

$$\hat{P}_a^z = \hat{P}_T/P_a^z$$

3.14.7 Region and Group Balance Integral Components

1. Principal Balance Integral Components

For each of the three balance options (e.g. by region, by group or by region and group) the principal balance components

$$B_r^g = L_r^g + I_r^{a,g} + I_r^{o,g} - I_r^{i,g} - \frac{1}{k_{eff}} I_r^{f,g} - S_r^g \qquad (3.26)$$

are edited first and are defined below. The variety of integral forms available will only be listed for the balance term. The corresponding forms for each principal component is obvious:

$$B_a^g = \sum_{r\epsilon a} B_r^g, \quad B_T^g = \sum_r B_r^g$$

$$B_r = \sum_g B_r^g, \quad B_a = \sum_{r\epsilon a} B_r, \quad B_T = \sum_g B_T^g$$

a. Net Leakage

$$L_r^g = \sum_{n=1}^{4} L_r^{g,n}$$

The $L_r^{g,n}$ are defined later in this section.

b. Absorption (Capture + Fission)

$$I_r^{a,g} = \Sigma_r^{a,g}\phi_r^g$$

c. Outscatter (Removal - Absorption)

See Table 3.1 for a definition of the removal cross section.

$$I_r^{o,g} = (\Sigma_r^{r,g} - \Sigma_r^{a,g})\phi_r^g$$

d. Inscatter Source

$$I_r^{i,g} = \sum_{g'\neq g} \Sigma_r^{s,gg'}\phi_r^{g'}$$

e. Fission Source

$$I_r^{f,g} = \chi_r^g \sum_{g'=1}^{G} \nu\Sigma_r^{f,g'}\phi_r^{g'} \qquad \text{(Real)}$$

$$I_r^{f,g} = \nu\Sigma_r^{f,g} \sum_{g'=1}^{G} \chi_r^{g'}\phi_r^{g'} \qquad \text{(Adjoint)}$$

f. External Source (Inhomogeneous problems only)

$$S_r^g = W_r \sum_{ijk\varepsilon r} S_{ijk}^g V_{ijk}$$

2. Leakage and Buckling Components

In any problem the net leakage (item 1a. above) is defined by up to three directed leakage components corresponding to the problem coordinate directions. $L_r^{g,4}$ denotes an optional DB^2 leakage term applicable to one- or two-dimensional problems. The $L_r^{g,n}$, n=1,2,3 are defined by

$$L_r^{g,n} = \sum_{ijk\varepsilon r} L_{ijk}^{g,n}$$

where the mesh cell leakage components $L_{ijk}^{g,n} \equiv L_\ell^{g,n}$ are defined by

$$L_\ell^{gn} \equiv J_\ell^{2n} A_\ell^{2n} + J_\ell^{2n-1} A_\ell^{2n-1} \qquad n=1,2,3$$

see the definitions of J_ℓ^n and A_ℓ^p in Eq. (2.15) and Table 2.2, respectively.

In triangular geometry the $L_r^{g,1}$ term includes leakage components from both "X" and "Y" directions. $L_r^{g,1}$ is therefore replaced by the more useful planar leakage given by $L_r^{g,1} + L_r^{g,2}$. The quantity $L_r^{g,2}$ is also editted, but probably has limited use since it does not represent the entire "Y" leakage component.

By convention the DB^2 leakage term always uses $D_r^{g,3}$ (see Section 3.6.8) so that

$$L_r^{g,4} \equiv D_r^{g,3}(B^2)_r^g.$$

The leakage components $L_r^{g,n}$ may be used to define effective region bucklings

$$(B^2)_r^{g,n} \equiv \frac{L_r^{g,n}}{D_r^{g,n}\phi_r^g}, \qquad n = 1,2,3. \tag{3.26}$$

3. Miscellaneous Edits

a. Capture Rate

$$I_r^{c,g} = (\Sigma_r^{a,g} - \Sigma_r^{f,g})\phi_r^g$$

b. Fission Rate

$$F_r^g = \Sigma_r^{f,g}\phi_r^g$$

The following components are found on the group-integrated edits only.

c. (N,2N) Source

$$I_r^{N2N} = I_r^o - I_r^i$$

d. Net production

$$I_r^p = \frac{1}{k_{eff}} \sum_{g=1} I_r^{f,g} + I_r^{N2N}$$

The next three median energy edits use the following definitions:

$I_r^{s,g}$ = the type s reaction rate or flux integral

E_g = the maximum energy bound (ev) for group g

ℓ_g = $\ln (E_1/E_g)$ = lethargy for group g

The median energy of the type s integral is defined by

$$E_r^s = E_1/e^{\ell_{g'}+\alpha(\ell_{g'+1}-\ell_{g'})} \tag{3.27}$$

where

$$\alpha = \frac{1}{2} I_r^s - \sum_{g<g'} I_r^{s,g} \tag{3.28}$$

$$g' = \left\{ \min g \;\middle|\; \sum_{g''<g+1} I_r^{s,g''} > \frac{1}{2} I_r^s \right\}. \tag{3.29}$$

The following three median energy integrals may then be defined using Eqs. (3.27)-(3.29).

e. Median Energy of Fission Source

$$E_r^f, \text{ let } I_r^{s,g} = I_r^{f,g}$$

f. Median Energy Absorption Rate

$$E_r^a, \text{ let } I_r^{s,g} = I_r^{a,g}$$

g. Median Energy of Total Flux

$$E_r^\phi, \text{ let } I_r^{s,g} = \phi_r^g.$$

3.15 Signs of Trouble

3.15.1 Error Messages

During the processing of input data an effort is made to detect as many user errors as possible in a single job. To this end, fatal errors are recorded and printed as they occur, but in many situations processing is resumed until the currently executing module completes its tasks. Non-fatal warning messages may occur from time to time indicating situations that may be suspect, and therefore warrant the users attention.

A typical case in point occurs when DIF3D iterations are prematurely terminated because the outer iteration limit has been exceeded. Here the message is intended to simply remind the user that the specified convergence has not been achieved.

The warning message advising that the iteration threshold has been reached during the optimum overrelaxation factor calculation frequently occurs in applications for which the spectral radii of the inner iteration matrices are close to unity, as is frequently the case in thermal reactor problems. In practice this message is no cause for alarm, but simply reflects the fact that the convergence test in Eq. (2.94) is too stringent.

Reactor models with steep flux gradients near reactor boundaries (research reactors are a good example here) frequently trigger underflow error messages during the calculation of optimum overrelaxation factors. The error message simply reflects the fact that some of the mesh cell fluxes that are involved in a squaring operation are extremely small. The message may be ignored, since the offending fluxes have a negligible contribution to the norms being calculated. However, it should be clear that such pathological situations are the cause of the messages and not some more basic difficulty in problem specification.

3.15.2 Non-monotonic Convergence

Other than convergence criteria, the only parameter the user has at his disposal to influence the DIF3D outer iteration process is the inner iteration error reduction factor which may be supplied on the Type 06 card of A.DIF3D.

When the user has specified a factor that is too "loose", the pointwise fission source monitor on the outer iteration history page undergoes erratic behavior. In extreme cases iterations may reach a point after which no further progress is made. When such behavior is observed it is useful to take note of the dominance ratio estimates which also appear in the iteration history edit. If these are erratic or exceed unity, it is a sign that the inner iteration error reduction factor must be "tightened" (i.e. reduced in magnitude).

The effects of increasing and decreasing (by powers of 4) the error reduction factor (ϵ_{in}) is illustrated in Tables 3.6-3.8 for three reactor models. In a given model, the container storage remained fixed for all ϵ. Consequently, EXCP charges and job cost are not optimized in cases involving the concurrent inner iteration strategy (i.e. the optimal CITS bandwidth changes as the number of inner iterations change). The results indicate that 0.04 is at best conservative (i.e. in these problems there is no incentive to tighten the error reduction). On the other hand if the user plans to run a series of similar models, it will likely be to his advantage to attempt further cost reduction by first loosening the error reduction (increasing ϵ_{in}), then adjusting the DIF3D ECM container size to a value which yields the optimum inner iteration bandwidth for this problem.

TABLE 3.6. Inner Iteration Error Reduction Effects for the SNR Benchmark Problem[a]

g	ω_g	$m_g(.64)^b$	$m_g(.16)^b$	$m_g(.04)^b$	$m_g(.01)^b$	$m_g(.0025)^b$
1	1.45386	3	6	8	10	12
2	1.60581	5	9	12	15	18
3	1.32388	3	4	6	7	9
4	1.40978	3	5	7	9	11
NO. INNERS/OUTERS		14	24	33	41	50
TOTAL OUTERS ($\epsilon_\lambda=10^{-5}$)		39	20	17	15	15
TOTAL INNERS		546	480	561	615	750
CPU SEC. (195)		40	32	34	34	40
EXCP		2745	2745	2713	2710	2737
COST		$8.11	$7.00	$7.21	$7.25	$8.06

[a] 4 group 31 × 16 × 18 sixth-core model of the original triangular-geometry SNR benchmark problem (see Section 5.3.1).

[b] $m_g(\epsilon_{in})$ is the number of inner iterations in group g required to achieve an error reduction factor of ϵ_{in}.

TABLE 3.7. Inner Iteration Error Reduction Effects for the LCCEWG Benchmark Problem[a]

g	ω_g	$m_g(.16)$[b]	$m_g(.04)$[b]	$m_g(.01)$[b]
1	1.59915	8	11	14
2	1.66320	10	14	17
3	1.60623	8	12	15
4	1.65964	10	13	17
NO. INNERS/OUTER		36	50	63
TOTAL OUTERS (ϵ_λ=10^{-4})		27	23	22
TOTAL INNERS		972	1150	1386
CPU SEC. (3033)		273	315	349
EXCP		38339	40443	42261
COST		$44.68	$49.62	$53.59

[a] 4-group 49 × 25 × 28, sixth-core model of the LCCEWG benchmark BOL problem.[28]

[b] $m_g(\epsilon_{in})$ is the number of inner iterations in group g required to achieve an error reduction factor of ϵ_{in}.

TABLE 3.8. Inner Iteration Error Reduction Effects for a ZPPR 11(B) Model[a]

g	ω_g	$m_g(.16)$[b]	$m_g(.04)$[b]	$m_g(.01)$[b]
1	1.71197	12	17	22
2	1.73051	13	18	24
3	1.75589	15	21	26
4	1.76420	15	21	27
5	1.76339	15	21	27
6	1.74382	14	20	25
7	1.74804	14	20	25
8	1.76436	15	21	27
9	1.74110	14	19	25
NO. INNERS/OUTER		127	178	228
TOTAL OUTERS (ϵ_λ=10^{-5})		25	23	23
TOTAL INNERS		3175	4094	5244
CPU SEC. (195)		115	130	153
EXCP		15650	14787	14795
COST		$23.02	$24.14	$26.22

[a] 9 group 60 × 120 half-core ZPPR 11(B) model.

[b] $m_g(\epsilon_{in})$ is the number of inner iterations in group g required to achieve an error reduction factor of ϵ_{in}.

3.16 Special DIF3D Applications

The following sections are brief outlines of some of the special applications of DIF3D available at Argonne. These are not available in the export version of the code; they are included in this report primarily to stimulate users to use the code in unique and creative ways. Some of the special applications make use of one or more of the four user modules UDOIT1 - UDOIT4 which are discussed in Section 4.1.11, (see also Fig. 1.1).

3.16.1 Perturbation Theory - VARI3D

VARI3D[14] is a set of code blocks currently under development in the Applied Physics Division for doing ordinary and generalized perturbation theory calculations. Many of the code blocks and files described in this report are also used in VARI3D. Additional code blocks have been written to set up direct and adjoint DIF3D calculations, to calculate inner products and to edit the perturbation results.

3.16.2 Fuel Cycle Analysis - REBUS-3

REBUS-3[7] is a set of code blocks currently under development in the Applied Physics Division for doing fuel cycle analysis for one-, two- and three-dimensional diffusion theory models. Many of the code blocks and files described in this report are also used in REBUS-3. Additional code blocks are being written to set up DIF3D calculations and to calculate the burn-up.

3.16.3 Calculating Higher Harmonics

DIF3D has been used a number of times to calculate higher harmonics of the one-, two- and three-dimensional neutron-diffusion finite-difference equation.

The UDOIT2 dummy code block, which is executed just prior to the DIF3D solution code block, is replaced by a program which generates and saves a flux guess which contains all harmonics; this is currently done using a random number generator.

Next, fundamental mode direct and adjoint flux solutions are run with tighter than usual convergence criteria. The UDOIT3 position, just after the DIF3D solution code block, is used for a program which strips the fundamental mode from the original flux guess using the orthogonality condition for eigenfunctions.

The path of the calculation then loops back to the DIF3D solution code block for a few outer iterations, after which the latest flux iterate is again purged of the fundamental by the UDOIT3 coding. This loop continues until the second and higher harmonics have been iterated out of the flux. If the first harmonic flux and adjoint are calculated in this way the UDOIT3 coding can be made to drive second harmonic calculations.

DIF3D can calculate harmonics because it uses a linear acceleration scheme that cannot reintroduce large components of the fundamental into the flux iterate. The fundamental does grow back into the flux iterate (therefore the succession of purges), but it does so starting from the level of the convergence of the original flux and adjoint problems. Periodic purging easily keeps it in check.

In this application of DIF3D the only programming involved is in the UDOIT2 and UDOIT3 positions. The remainder of the code is used without internal changes.

3.16.4 Calculating Electrostatic Potential Distributions

DIF3D has been used on one occasion to solve for the electrostatic potential distribution in a relatively complicated system of conducting electrodes and dielectric material. DIF3D does not permit internal, inhomogeneous (fixed-potential) boundary conditions of the sort needed for electrostatics, but this difficulty was overcome by a Green's function approach and the UDOIT feature of the code.

The electrodes, on which fixed potentials are to be applied, are divided into regions small enough that the internal charge distributions can be approximated by a constant. A "multigroup" cross section set (A.ISO) of one isotope is set up with no group-to-group transfer, no removal or fission and unit transport cross section. The dielectric constant for various regions can then be set by adjusting the number density input for each region of the model. A fixed source (FIXSRC file) is generated, each group of which has a unit source in a different, individual electrode region and a zero source elsewhere. One solution of this "multigroup" fixed source problem yields the simultaneous solution for the complete set of Green's functions, one for each electrode region.

The overall potential distribution in the model is the sum of products of each Green's function distribution times a charge-density multiplier for the corresponding electrode region. An additional program was written for the UDOIT3 position in the code to calculate the multipliers for each Green's function (i.e. each electrode region). A least-squares criterion was applied to minimize the difference between the Green's function solution and the applied voltages in the electrode regions.

In this application of DIF3D the only programming involved was in the UDOIT3 position. The remainder of the code was used without internal changes.

3.16.5 Neutron Transport with Isotropic Scattering

A version of the DIF3D code block has been modified at Argonne to perform S_n transport calculations for isotropic scattering. The diffusion-theory equation coefficient and solution routines were replaced by transport theory counterparts for two-dimensional X-Y, R-Z and triangular geometries. Although this still must be considered an experimental code, DIF3D/transport is used quite regularly in the analysis of critical experiments and in core design applications. Its main advantage over other available transport codes is that its input is identical to the standard, diffusion-theory version of the code, which is a considerable convenience to analysts at Argonne.

4. PROGRAMMING INFORMATION

This chapter contains detailed programming information concerning the overall structure and function of the major code blocks in the DIF3D system. The information is primarily intended for the programmer concerned with DIF3D source code modifications and for users who wish to understand particular details of the calculational flow. Additional details are provided by internal code documentation included in the DIF3D source code.

4.1 Role and Function of Subprograms

The DIF3D system consists of a collection of large independent code blocks logically connected by a small "driver" subroutine D3DRIV (standard path STP021 in ARC System terminology). D3DRIV dynamically invokes the code blocks according to data-dependent logic. The code blocks communicate with each other, and with D3DRIV, by means of interface files; with the exception of the three utility routine COMMON blocks mentioned in Section 4.1.1, no data are passed in-core from one code block to another.

DIF3D is carefully designed to run in one of two different environments: modular and standalone. In the modular format each code block, including STP021, is organized as a separate load module. Each load module contains versions of all the utility subroutines called from the module and is, in fact, an executable program. At Argonne, and at other IBM installations at which Argonne staff maintain codes, DIF3D is set up in modular style.

In the standalone format the entire production code is a single load module. D3DRIV and the utility subroutines are contained in the root overlay; the code blocks executed by D3DRIV are separate overlays. The National Energy Software Center versions of DIF3D are set up in standalone style (see Chapter 5).

4.1.1 Module and Overlay Driver - STP021 (D3DRIV)

D3DRIV (STP021) is a small driver subroutine that controls the load module (overlay) calculational sequence ("path") in all DIF3D problems. Figure 1.1 illustrates the sequence of module calls in D3DRIV and the input and output datasets employed by each module. (See Table 4.2 for a detailed list of input and output data sets for each module). Module execution is initiated via the LINKER0 or LINKER1 subroutines described below.

The path has a simple loop structure which permits multiple case problem sets; modules in the path are conditionally executed based on the existence of interface files. Within the case loop there exists a search loop which is only triggered by the existence of the SEARCH interface file. Termination of the search loop is triggered by a sentinel on the SEARCH file.

The file "existence" attribute is obtained via calls to the CCCC utility subroutine SEEK (see the discussion in section 4.3.4.1). These dynamic attributes are maintained by SEEK and changed by modules in the course of problem execution. Prior to invoking the first module, D3DRIV initializes subroutine SEEK by passing to it a list of file names (DSNAME array) and a corresponding list of logical unit number assignments (NREF array). It must also initialize the COMMON blocks IOPUT, PTITLE and STFARC, which are required by certain of the utility subroutines.

The logical unit numbers (NIN, NOUT and NOUT2) for the card-input and the two printer-output files are defined and stored in COMMON block /IOPUT/. They are also stored in COMMON block /PTITLE/. The page heading information and timing information in /PTITLE/ are frequently reinitialized upon entry to a new module. Initialization of COMMON block /STFARC/ is described in the discussion of the SCAN module in the next section.

Subroutines LINKER0 and LINKER1 were written to simplify the readibility and programming of D3DRIV. The subroutines are identical in coding; separate names are required to prevent recursion. Their function is to provide the module calling sequence appropriate to the modular or stand-alone environments. In a modular environment on IBM/370 systems execution is transferred to load modules via the LINK[36,41] macro. In a stand-alone system the appropriate overlay call is generated. Auxiliary functions including elapsed time of module execution and (in the ANL modular system) the detection and listing of logical unit numbers left open upon module exit, are also provided.

4.1.2 Input Preprocessors - SCAN and STUFF

The two code blocks which preprocess the BCD card input file are SCAN and STUFF. This section discusses their use in a program (see also Ref. 41).

SCAN must be called before any BCD input is read and before the first call to STUFF; it is called only once in a job. The initialization call to SEEK must precede the call to SCAN. SCAN reads the entire BCD card input file from logical unit NIN (NIN is the first variable in the labeled common block /IOPUT/) and copies it to another file which is either the file named ARC or, if ARC is not in the SEEK tables, logical unit 9. In the process it sets up a table of pointers to the beginning of each BLOCK. The call to SCAN also processes the data in BLOCK=OLD if that block is present in the input file.

All BLOCKs other than BLOCK=OLD are processed by calls to STUFF. Before each call to STUFF the variable STFNAM (the first variable in the labeled common block /STFARC/) must be set equal to the name of the BLOCK to be processed. For the DIF3D code that name is "STP021". STUFF returns a flag (NRET in /STFARC/) which permits the program to test for end of input. STUFF writes, or rewrites, each BCD disk file referenced under the particular BLOCK=STFNAM according to the instructions in the input (DATASET=, MODIFY=, etc.). It is STUFF that reorders, replaces and deletes numbered cards. Since the STUFF processing follows the processing of BLOCK=OLD by SCAN, a new DATASET input on cards would destroy the data already on an existing file of the same name referenced under BLOCK=OLD.

Figure 4.1 shows a simple driver that uses SCAN and STUFF to preprocess BCD card input. In fact, this driver could be used with the input shown in Figure 3.1 since the BLOCK and DATASET names are consistent. The driver starts by setting card and printer file numbers and by initializing SEEK, TIMER and LINES. Following the single call to SCAN it goes into a loop containing a call to STUFF and an execution of a program (PROG). Execution terminates when the last BLOCK=TEST has been processed. Figure 4.1 is a simplified, but otherwise typical, driver; a calculation is performed for each BLOCK in the input.

As it writes or rewrites a BCD card image file STUFF inserts a few formatted records at the beginning which contain information about the structure of the file. These lead records may be read:

```
CSW
      IMPLICIT REAL*8(A-H,O-Z)
CSW
      COMMON /PTITLE /TITLE(66), TIME(10), HNAME(4), KOUT, KOUT2, NTITLE
      COMMON / IOPUT / NIN, NOUT, NOUT2
      COMMON / STFARC / STFNAM, BLKNAM(50), IBLTAB(3,50), NBLOCK, NRET
      DIMENSION DSNAME(6)
      DATA DSNAME / 8HA.SAMPLE, 8HA.SAMPLE, 8HA.XAMPLE, 6HRTFLUX,
     1 6HISOTXS, 1H$ /
      DATA BLOCK/4HTEST/, BLANK/6H      /
      DATA IM1/-1/, I0/0/, I1/1/, I3/3/, I4/4/, I11/11/
C
      NIN=5
      NOUT=6
      KOUT=NOUT
      NOUT2=I0
      KOUT2=NOUT2
      NTITLE=0
C
C     INITIALIZE TITLE AND HNAME TO BLANKS
C
      CALL FLTSET(TITLE,BLANK,I11)
      CALL FLTSET(HNAME,BLANK,I4)
C
      N=0
      CALL SEEK(DSNAME,I1,N,I3)
      CALL TIMER(I0,TIME)
      CALL TIMER(IM1,TIME)
      CALL LINES(I0,I)
      CALL SCAN
C
      STFNAM=BLOCK
   10 CONTINUE
      CALL STUFF
      IF( NRET.LE.0 ) GO TO 20
      CALL PROG
      GO TO 10
C
   20 CONTINUE
      RETURN
      END
```

Fig. 4.1. An Example of the Use of SCAN and STUFF

```
      READ(M,99)ANAME,MAXTYP,NONUM,NOFORM,(N(I),I=1,MAXTYP)
   99 FORMAT(A8,3I5/(16I5))
```

M	file logical unit number
ANAME	file name
MAXTYP	highest card type number in file
NONUM	number of unnumbered cards
NOFORM	0/1, cards are to be read formatted/free-format
N(I)	number of cards of type I

The logical unit number, M, should be obtained through calls to SEEK and SEKPHL:

```
      CALL SEEK(ANAME,IVER,I,0)
      CALL SEKPHL(I,M,0)
```

IVER	file version number
I	file reference number

There are always at least two of these lead records in a BCD file written by STUFF; FORTRAN I/O expects a second record even if MAXTYP=0. Indeed, for NOSORT DATASETs MAXTYP is zero.

The NOFORM sentinel is 0 for files designated DATASET= or SUBLOCK=; it is 1 for files designated UNFORM=.

These lead records permit applications modules reading BCD files to make decisions based on the presence or absence of particular card types. The user's input card images follow the lead records and can be read as if they were cards - one 80-column card per record.

4.1.3 CSE010 (ANL only)

CSE010 converts cross section data from the ARC System (XS.ISO) file36 format to the CCCC isotope ordered file format (ISOTXS). The code will also merge two ISOTXS files into a single output file. CSE010 is made up of five subprograms and is not overlayed. The entry routine CSE010 allocates the BPOINTER container array and calls the various subroutines to perform their specific tasks. The input files used by CSE010 are XS.ISO, the input ARC System double precision cross section file, ISOTX1 and ISOTX2, the input CCCC files which may be merged into the final output ISOTXS file. There is no BCD input to the routine. Following problem setup the subroutine CTAD is called to load isotope independent data from the XS.ISO file into appropriate arrays. PRINXD is then called in a loop over isotopes to process the isotope cross sections from the XS.ISO file. Since the ARC System file contains derived data rather than the specific cross sections required in the ISOTXS file, an approximation is required in deriving the CCCC data. In particular, it is assumed that the flux and current weighted total cross sections are equal. This approximation allows a unique conversion of the XS.ISO data to an ISOTXS format. If input ISOTXS files ISOTX1 and/or ISOTX2 are available, the subroutines ISOCTL and PRINO are called to add these data to the data generated from the XS.ISO conversion.

4.1.4 LASIP3 (ANL only)

The LASIP3 module[37] was developed at Los Alamos for processing Version-3 standard CCCC interface data files. It performs two distinct tasks; namely

transforming free-field format, BCD data into well-defined binary files and providing for printing and punching data in the binary files.

LASIP3 is impleme ted in the modular environment on the IBM 370/195 at Argonne to provide auxiliary input processing capabilities of interest to a limited number of DIF3D users. It is not implemented in the NESC versions of DIF3D detailed in Chapter 5.

LASIP3 was modified to incorporate the dynamic storage allocation capability provided by the BPOINTER package discussed elsewhere in this document, thereby eliminating a fixed length working storage array previously required in LASIP3 (see sample input in Fig. 3.7).

4.1.5 The General Input Processor - GNIP4C

GNIP4C is an input processor that generates a number of CCCC Standard Interface Files from BCD card-image input. Figure 4.2 shows the structure of the code. The main driver (GNIP4C) calls on one or more of nine subprograms.

The combination of subprograms RANIP1 and FGEODS reads geometry data from A.NIP3 cards and generates a GEODST file. For the most part RANIP1 reads and checks the data, and FGEODS composes the GEODST and LABELS files. All subroutines in GNIP4C whose names start with "ANIP" (e.g. any of the routines in RANIP1) read one (and occasionally two) card types. If a GEODST file is input RANIP1 and FGEODS are skipped.

The third subprogram, EGEODS, edits the GEODST file at the user's request. EGEODS contains graphics and printer output routines that generate maps of arrays of hexagons (TRIPLT) or orthogonal geometries (ORTMAP). TRIPLT uses data from the A.NIP3 type 15 and 30 cards, and so GNIP4C is not able to generate hexagonal array maps when the geometry is input via a GEODST file. ORTMAP generates its maps from data in the GEODST file. There is coding in the subroutines associated with TRIPLT and ORTMAP to generate computer graphics maps via standard CALCOMP or DISPLA calls. This coding is commented out in the NESC versions of the code, but it is not difficult to reactivate.

RANIP2 and FADENS read A.NIP3 data and write the number density files (NDXSRF and ZNATDN). Number density edits are produced as the input data are processed from A.NIP3 into GEODST, and so it is not possible for GNIP4C to edit atom densities when they are input to the code in the ZNATDN file. RANIP2 and FADENS are skipped entirely if NDXSRF and ZNATDN already exist.

BCDXST reads the formatted version of the ISOTXS file from a NOSORT DATASET named A.ISO. This is the only direct means by which the user can input cross sections to the code on cards. BCDXST converts the formatted, BCD form into the binary file ISOTXS. Coding exists in the subprogram to convert in a similar way a formatted version of the delayed neutron data file DLAYXS[6] to a binary form, however, the delayed neutron file names have not been included in the DIF3D SEEK tables. There are internal flags in BCDXST which trigger edits of ISOTXS and DLAYXS; however, these flags cannot be manipulated from outside the code.

The seventh subprogram, WRSORC, reads inhomogeneous source specifications from A.NIP3 cards and generates and edits a FIXSRC file. WRSORC is skipped when none of the fixed source card types (A.NIP3 19 and 40-42) appear in the input.

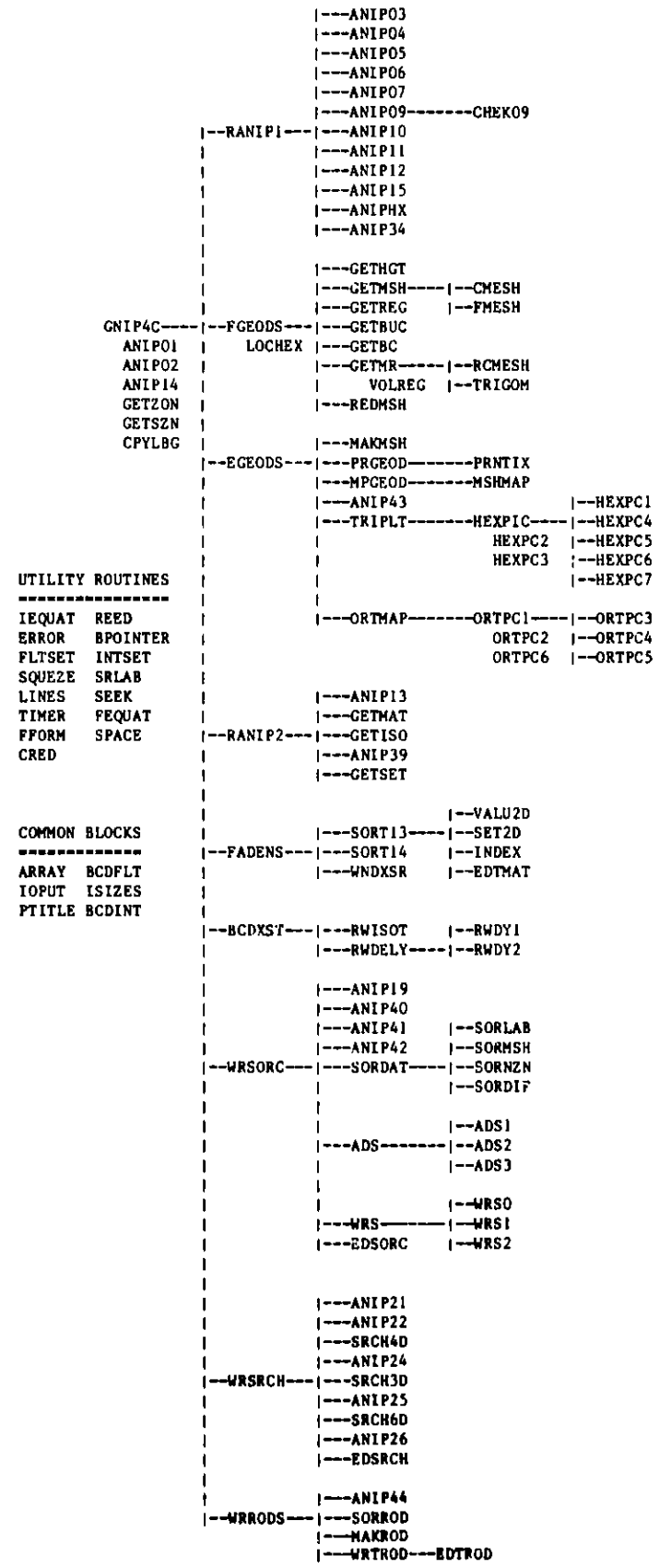

Fig. 4.2. Subroutine Map for the GNIP4C Code Block

WRSRCH reads specifications for the criticality search option and writes and edits the SEARCH file. WRSRCH is skipped when none of the search card types (A.NIP3 21-26) appear in the input.

WRRODS processes the input for the control rod model and it is skipped when the A.NIP3 type 44 cards are absent.

4.1.6 Cross Section Homogenization - HMG4C

HMG4C is a cross section processor which generates the macroscopic cross section file COMPXS based on the data contained in the CCCC files ISOTXS, NDXSRF, ZNATDN, and DLAYXS. In generating the macroscopic data, it is assumed that there is a one-to-one correspondence between compositions and zones. Thus, for example, the fifth composition on the completed COMPXS file corresponds to the data for zone number five on the two CCCC files NDXSRF and ZNATDN. The code accepts the CCCC files in their full generality with the single exception that an isotope or file-wide CHI matrix is not permitted.

The data management strategy used by the code is rather straightforward. After reading and storing the data obtained from the ZNATDN and NDXSRF files, and the isotope independent data of ISOTXS and DLAYXS, the code attempts to hold all of the fourteen different types of macroscopic array data in the remaining container space. If this is possible then a single pass is made through the ISOTXS file and the contribution of each relevant isotope is added to each macroscopic cross section of each composition. If all the macroscopic arrays will not fit in the available core, the code determines the maximum number of compositions which can be homogenized in a single pass. As many passes are then made as required to completely process the data. The results of each pass are written on a scratch file (SCR001) for temporary storage before being rewritten to the COMPXS file.

The three CCCC files ISOTXS, NDXSRF, and ZNATDN are always required input to HMG4C and hence must be declared under a BLOCK=OLD statement in the input data or generated from input BCD data by the code block GNIP4C. The file DLAYXS is optional but must be included under BLOCK=OLD if delayed neutron data are required. Additionally, the user may specify the BPOINTER container size, the method by which the composition fission spectra are to be computed, and various edit options on the BCD dataset A.HMG4C.

Figure 4.3 shows the structure of the code. The subroutines of HMG4C may be divided into four separate functional units of code each of which may be linked to form a separate overlay. The first overlay, OVL1, reads all of the input data except for the microscopic cross sections. The second overlay, OVL2, computes the homogenized cross sections in the form of fourteen macroscopic arrays which are the working storage units of the code block. In the third overlay, OVL3, the COMPXS data set is written from the data contained in the fourteen working arrays. The fourth overlay, OVL4, is essentially independent of the preceding three and is used to edit a COMPXS file. HMG4C may be used for the express purpose of editing a user input COMPXS file, in which case only the fourth overlay is executed.

4.1.7 MODCXS

MODCXS is an input processor that modifies an input macroscopic cross section file, COMPXS, to account for user specified directional diffusion coefficients and/or energy conversion factors. A COMPXS file generated by the

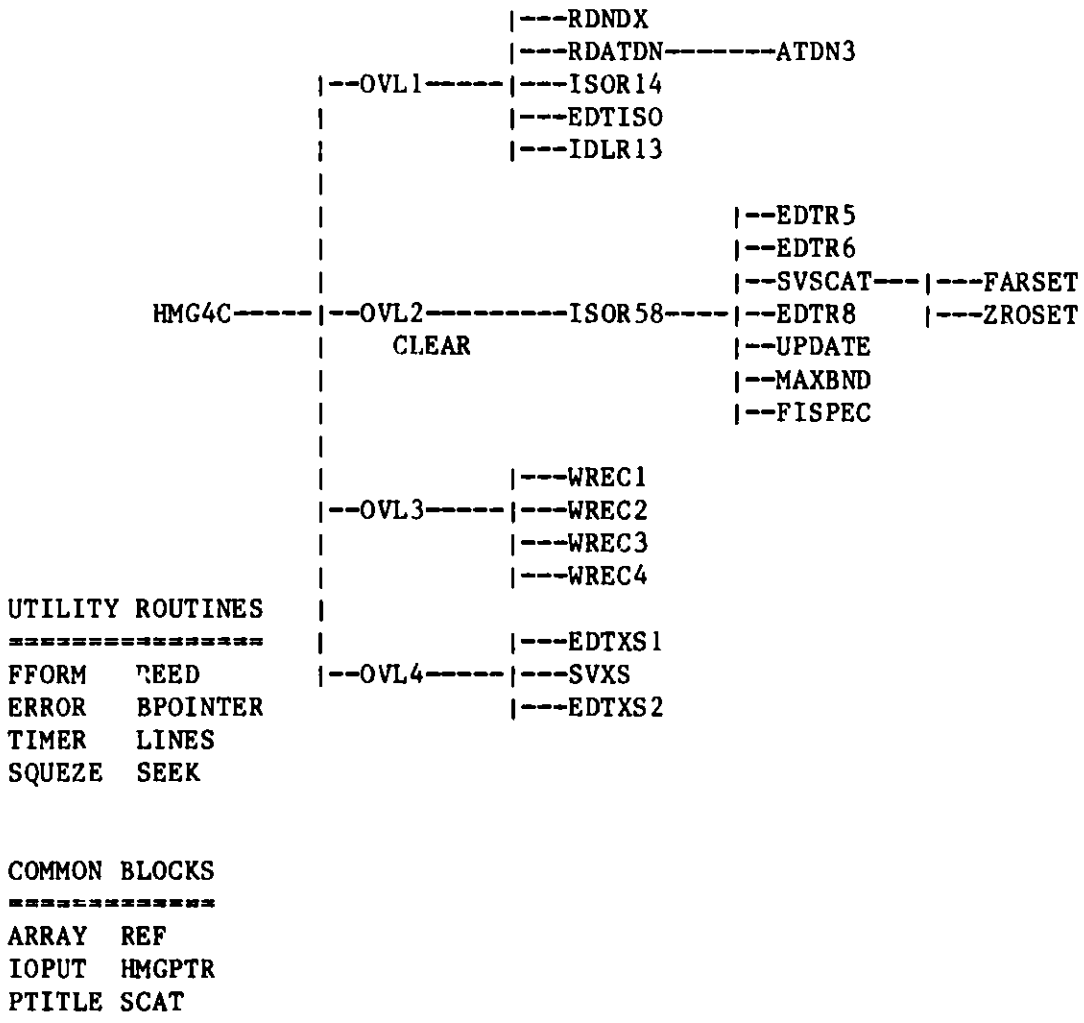

Fig. 4.3. Subroutine Map for the HMG4C Code Block

code block HMG4C does not include any directional diffusion coefficient capability. Furthermore, the fission and capture energy conversion factors are derived directly from the data available on the input ISOTXS cross section file. User input to override these data may be specified and the code block MODCXS processes these data.

The code block MODCXS is made up of five subroutines. The main driver MODCXS allocates the BPOINTER container for the code block and controls the program flow. The first program routine called by MODCXS is ANIP35 which reads and validates the directional diffusion coefficient data input by the user on the Type 35 and Type 36 cards of the A.NIP3 dataset. The subroutine ANIP37 is then called to read and validate the energy conversion factor data from the Type 37 and/or Type 38 cards of A.NIP3. The subroutine DOMODS is then called to process the user input data. DOMODS reads version 1 of the file COMPXS and writes the file SCR001 in the same format as the COMPXS file after modifying the power conversion and directional diffusion coefficient factors according to the user specifications. Finally the subroutine COPIER is called to copy the data from the file SCR001 onto the file COMPXS. The standard utility routines are used throughout the code block to ensure code standards.

4.1.8 BCDINP

BCDINP creates and modifies the DIF3D control file (also called DIF3D) from default values and/or from the BCD dataset A.DIF3D. BCDINP is comprised of three subroutines and is not overlayed. The driver subroutine BCDINP sets the A.DIF3D default parameters for the DIF3D file. If an old DIF3D file exists the default data is overridden by data read from the existing DIF3D file. If an A.DIF3D file exists, subroutine RADF3D reads A.DIF3D and updates the DIF3D file arrays with non-default data from A.DIF3D. Upon successful validation of the DIF3D file arrays by subroutine PDIF3D, BCDINP writes the interface file DIF3D.

4.1.9 SRCH4C

The SRCH4C module controls the criticality search iterative process by adjusting certain parametric vectors in order to achieve a desired value of k-effective. Search control information including the three most relevant search pass parameter estimates are maintained by SRCH4C on the CCCC interface file SEARCH (Appendix C.7). The interface files containing the parameter vectors appropriate for the selected search option are also modified by SRCH4C.

At the start of each search pass SRCH4C reads the SEARCH file to establish the search control parameters. Next the header records of interface datasets required for the selected search option are read and checked for data consistency. Subroutine GETCON performs this function in the concentration search option. Data management requirements for performing the interface file modifications in core-contained mode or with auxiliary disk storage are determined at this time. If the DIF3D file is present the BPOINTER ECM container size estimate is obtained to determine the feasibility of the core-contained option.

The most recent eigenvalue estimate will be read from the DIF3D file, if present, otherwise it will be taken from the RTFLUX file. Then subroutine SRCHX is invoked to calculate the new search parameter estimate based upon

the previous estimates. A parabolic extrapolation method with root-bracketting uses three recent estimates to accelerate the parameter search process. Upon completion of the two initial search passes with initial parameter estimates, one linearly extrapolated estimate is employed before the parabolic procedure is invoked. The search parameter is permitted to exceed its user specified range only once during the estimation algorithm. Subsequent occurences lead to problem termination.

Upon return from SRCHX the search history array is updated and the SEARCH file is rewritten. If the search parameter has not yet converged the subroutine which modifies the search quantity interface files is called. Subroutine DMDCON modifies the subzone volume fractions on the NDXSRF file for the concentration search option. Upon successful modification of NDXSRF, DMDCON turns off the COMPXS existence sentinel so that upon return from SRCH4C, subroutine D3DRIV will invoke HMG4C and MODCXS to obtain updated macroscopic cross sections.

SRCH4C has several features which exploit the time remaining feature of some systems and which exploit the DIF3D file if it is present. Consequently, the search is gracefully terminated if time limit is imminent. Abnormal termination of the DIF3D neutronics module is detected from the restart file DIF3D thereby causing SRCH4C to end gracefully and permitting a subsequent restart at the current search extrapolation cycle and/or at the next DIF3D outer iteration.

4.1.10 DIF3D

The DIF3D module performs the neutron flux and criticality calculations. Figure 4.4 illustrates the structure of the DIF3D module. Names preceded by asterisks in Fig. 4.4 are relevant only to the nodal solution option described in Ref. 5. They will not be discussed here. The four primary overlays called by DIF3D (BININP, SSINIT, SSTATE and DSSTOU) share COMMON blocks and BPOINTER FCM and ECM container arrays. Logic sentinels and problem specifications data reside in the /CONTRL/ and /SPECS/ COMMON blocks, respectively. Definitions for the elements of the COMMON blocks are located in subroutine BLOCKS which is included with the DIF3D source listing.

In stand-alone mode, the three-level overlay structure permitted by the CDC Overlay feature is retained by adding the DIF3D subroutine (and required utility subprograms) to the driver module D3DRIV. The different calling sequences required for the execution of DIF3D in a variety of computer systems in modular or standalone mode are unified via the subroutines LINKR0, LINKR1 and LINKR2. The suffixes 0,1 or 2 denote the (0,0)-, primary- and secondary-level overlay calls, respectively.

The module driver subroutine DIF3D initializes TIMER and then calls subroutine START which performs the following initialization functions:

1. Zeroes COMMON blocks;
2. Sets the machine dependent word length parameter LDW (=1 or =2);
3. Sets I/O mode parameters
4. Initializes units for BCD input and output files;

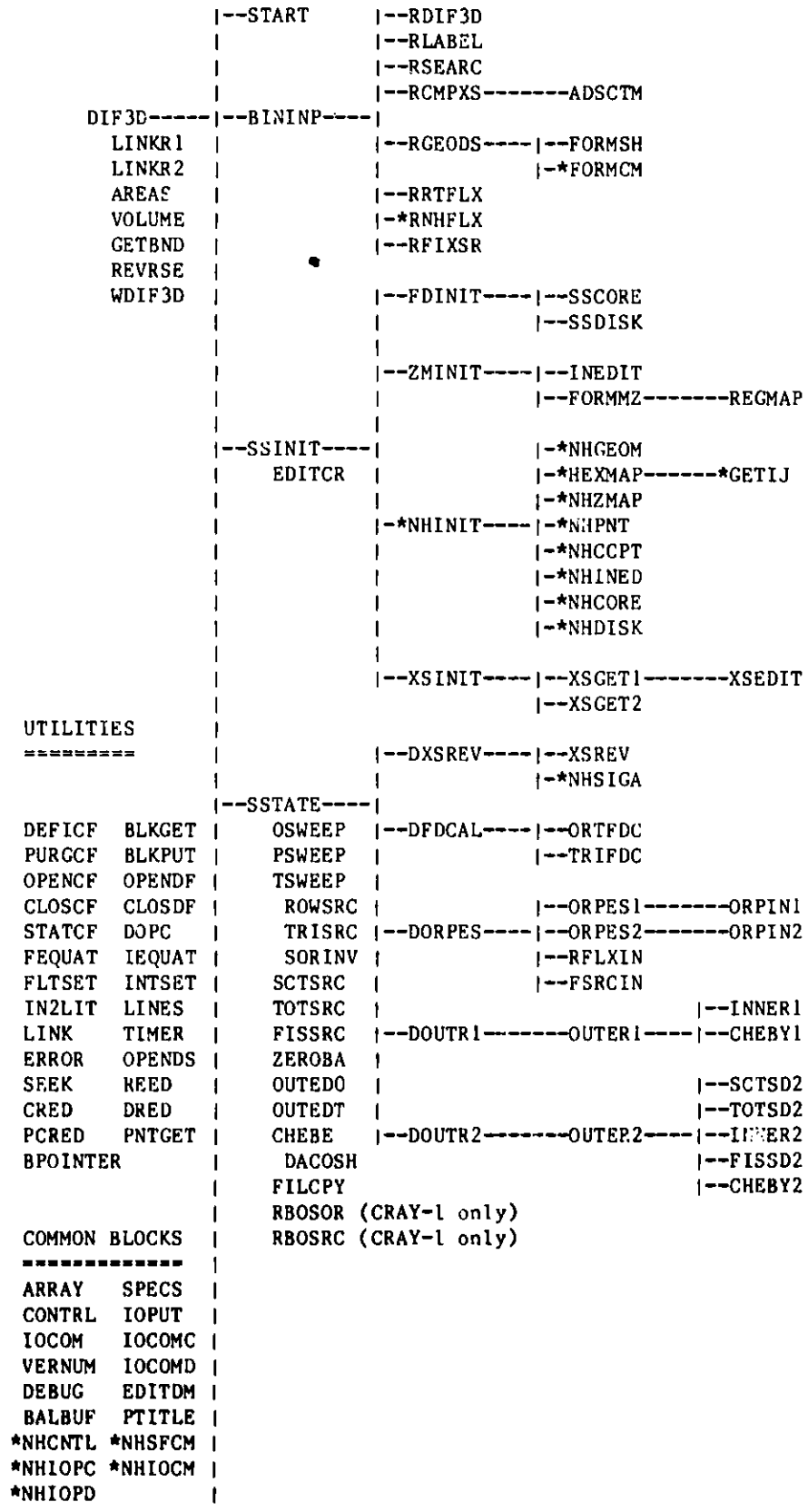

Fig. 4.4. Subroutine Map for the DIF3D Code Block

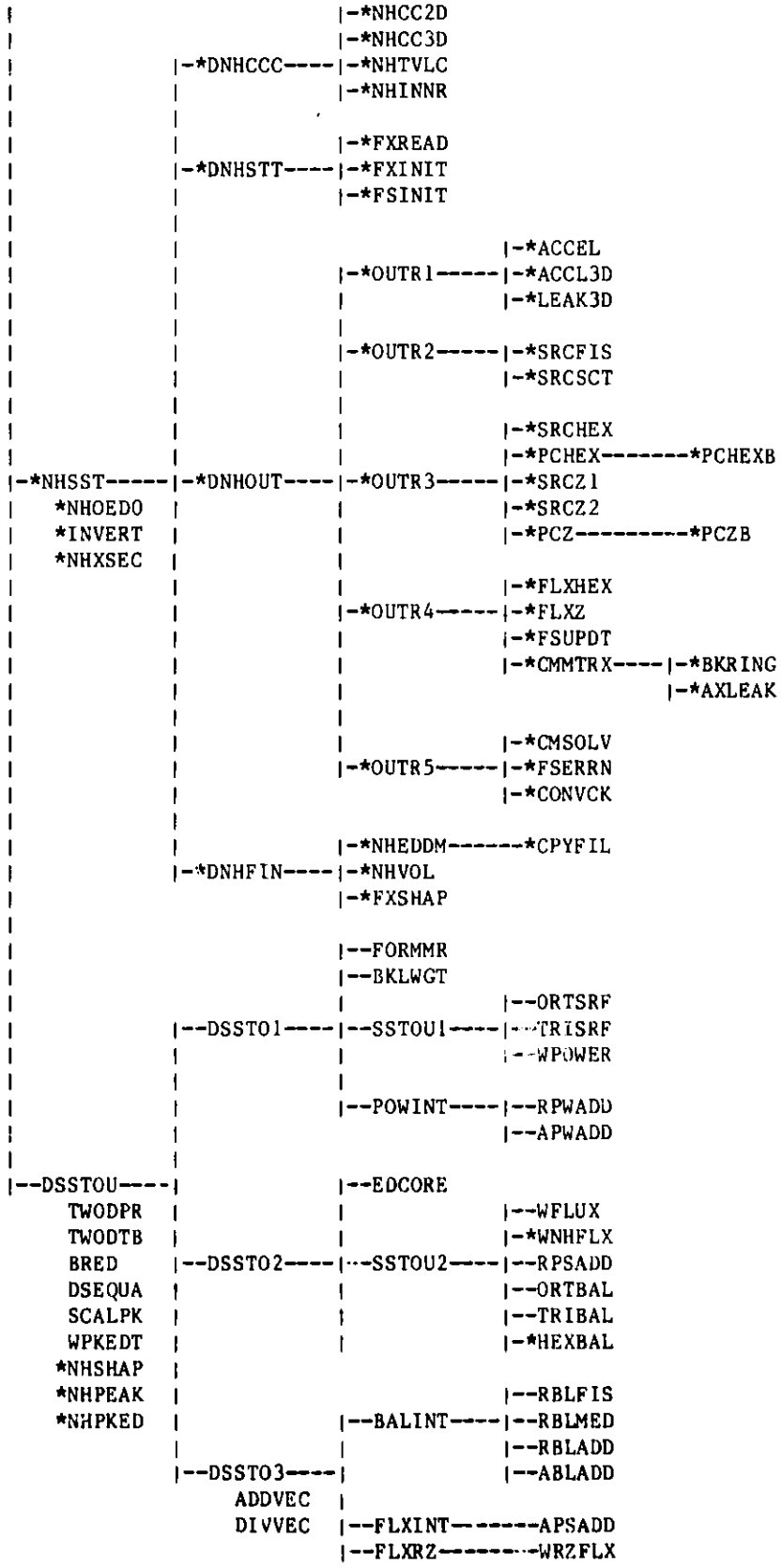

Fig. 4.4. Subroutine Map for the DIF3D Code Block (cont'd)

5. Reads BPOINTER container size data from the binary interface file DIF3D and allocates the container space.

Upon return from START, and prior to invoking the primary modules, DIF3D initializes the random access dataset utility routine DOPC.

The binary file input processor overlay driver, BININP, reads the specification records from the DIF3D input interface files listed in Table 4.2 (Section 4.2). The data is checked for consistency and entered into the pertinent COMMON block variables.

Using the data obtained in the BININP overlay, the SSINIT overlay calls SSCORE to determine the storage requirements for the DIF3D data manangement options. From these options SSCORE chooses the option that maximizes the usage of the available BPOINTER container space.

Upon completion of the data management edits in SSCORE, SSDISK is called to establish (via DOPC) the random access disk file group assignments required in the multilevel data management strategy. On CDC systems an auxiliary ECM container (see XCM discussion in Section 4.3.5.2) is allocated for storing the table of pointers that index the random access file records.

The problem input data and geometry description are edited by subroutine INEDIT. During the process of forming the zone map array, FORMMZ optionally calls subroutine REGMAP to edit the region and/or zone to mesh interval maps. If the zone map array cannot be ECM-contained in concurrent inner iteration problems, it is written to the random access scratch file ZONMAP.

XSGET1 reorders the group within composition (or zone) cross section data from the COMPXS interface file so that data is ordered by zone within cross section type for a given energy group. During this reordering process, XSGET1 computes directional diffusion coefficients and calls XSEDIT to edit the macroscopic cross sections. If the reordering process cannot be core-contained, cross sections are written by composition to the auxiliary file SCR001 by subroutine XSGET1. Subroutine XSGET2 performs the necessary number of read passes across SCR001 to complete the reordering process. In each pass a core-containable bandwidth of groups is processed.

The primary overlay SSTATE has five secondary overlays (DXSREV, DFDCAL, DORPES, DOUTR1 and DOUTR2). In adjoint problems, DXSREV calls XSREV which reverses the cross section group ordering and forms the adjoint scattering matrix. In the event that the available container storage is insufficient to core-contain all groups, the real problem cross sections are copied to auxiliary file SCR001. The cross section reversal process is then performed in multi-pass mode with the maximum permissible bandwidth of groups core-contained in each pass.

Overlay DFDCAL calls FDCAL which controls the finite difference coefficient calculation by calling the appropriate subroutines ORTFDC or TRIFDC for orthogonal or triangular geometries, respectively. For data management purposes, mesh cells for both orthogonal and triangular geometries are mapped by mesh plane onto a rectangular array. In certain triangular geometry problems and in problems with black absorber composition assignments some of

the mesh cells are excluded from the problem solution domain. In triangular geometry two arrays IS(j) and IE(j),j=1,2,...,J define the lower and upper index limits of the active mesh cells on line j. Mesh positions outside these limits are logically excluded from all calculations. Mesh cells which must be excluded from the problem domain, but which lie within the limits of the active mesh cells are effectively excluded from the problem domain by assigning the value zero to transverse direction coupling coefficients. Thus, computations proceed in an identical fashion for both active and excluded mesh cells with no additional logic overhead.

The DORPES overlay calls ORPES1 or ORPES2 to compute the optimum successive line overrelaxation factors for the inner (within group flux) iteration. Because of significant differences in data management strategy, dual sets of subroutines, differentiated by the suffixes 1 or 2, are employed. The first set applies to strategies in which at least one energy groups worth of data is ECM-contained; the second set applies to the concurrent inner iteration strategy which requires a minimum of three planes worth of data to be ECM-contained. Subroutines ORPIN1 and ORPIN2 control the Gauss-Seidel inner iterations employed to estimate the optimum factors ω_g. These routines were cloned from the routines INNER1 and INNER2 which perform the inner iteration sweeps during the outer iteration.

DORPES also calls RFLXIN and FSRCIN to read the real (adjoint) flux file RTFLUX (ATFLUX) and the fixed distributed inhomogeneous source file FIXSRC. If the the flux file does not exist, RFLXIN creates a flat flux guess of unity. In near-critical inhomogeneous source problems, an initial flux guess of zero is optionally generated. Mesh cells are initialized to zero when they are within the active portion of the rectangular data structure of the mesh plane arrays, but they are not part of the problem domain.

Overlay DOUTR1 calls subroutine OUTER1 which controls the outer (fission source) iterations and in thermal problems the upscatter iterations which are required to solve the multidimensional neutron diffusion equation when at least one energy group of flux, finite difference coefficients and cross section files can be ECM-contained. OUTER1 calls subroutines FISSRC, SCTSRC and TOTSRC which compute the fission, scattering and leakage sources and add them to the fixed source, if present. It also calls subroutines INNER1 and CHEBY1 which perform the inner iterations (within group flux calculations) and extrapolate the resulting fission source, respectively.

One of two data management strategies for calculating the scattering source are chosen based on whether or not the scattering band of fluxes can be ECM-contained. When the latter is true, the scattering source calculation is performed by double buffering the scatter band of fluxes through memory from disk one group at a time. When the former is true, the buffer for the scatter band of fluxes is treated in a circular manner. Upon filling the circular buffer, unneeded flux values are displaced, if necessary, by appropriate fluxes as the group index advances during each outer iteration.

Following each completed outer iteration pass, the average time required per outer iteration is computed to determine the feasibility of performing the next outer iteration and completing the editting wrapup in the remaining time indicated by the TIMER subroutine.

Overlay DOUTR2 calls subroutine OUTER2 which controls the outer iterations for the concurrent inner iteration option. The source computation routines (FISSRC, SCTSRC and TOTSRC) are called from the intermediate driver routines FISSD2, SCTSD2, and TOTSD2, respectively. The initial fission source is computed by IFISD2. Subroutines INNER2 and CHEBY2 perform the inner iterations and extrapolate the resulting fission source, respectively.

The scattering source calculation accesses blocks of flux planes from the energy groups in the scattering band of fluxes pertinent to the current energy group. The I/O requirements of such calculations are appropriately treated by the random access I/O features available on the IBM and CDC versions of DIF3D.

The DSSTOU overlay calls three secondary overlays (DSSTO1, DSSTO2 and DSSTO3) that perform the optional region, area and mesh cell flux integral edits. Two general purpose subroutines (TWODPR and TWODTB) are employed to perform mesh cell tabulations and region (and area) tabulations, respectively. TWODTB also writes a copy of the edited tables to the D3EDIT interface file.

The DSSTO1 overlay initializes the editting overlays by establishing the edit sentinels in COMMON block EDITDM and then calls FORMMR to generate the region-to-mesh-interval map array and BKLWGT to compute region-dependent transverse-direction weight factors for the volume and flux integrals. Subroutine SSTOU1 performs the following tasks:

1. Obtains the power normalization factor in real criticality (homogeneous) problems;

2. Edits and/or writes the PWDINT power density interface file;

3. Edits total power in real fixed source problems;

4. Controls the surface power and flux calculations in the ORTSRF and TRISRF subroutines;

5. Writes via WPKEDT the peak (surface) power interface file, PKEDIT, for the post processing edit module SUMMARY;

6. Edits maximum power density and corresponding mesh cell indices;

7. Creates the mesh cell power densities for subsequent use by the POWINT, RPWADD and APWADD subroutines which compute and edit the region and area dependent power density integrals.

The DSSTO2 overlay establishes via subroutine EDCORE the block sizes for the requested region and area integrals. Then subroutine SSTOU2 is called to write the appropriate flux interface files RTFLUX or ATFLUX. In real homogeneous problems the flux is power-normalized prior to editing or writing. The group-integrated fluxes by mesh cell are optionally edited here,also. If region or zone integral edits are requested, RPSADD is called to compute the region flux integrals. ORTBAL and TRIBAL are called to compute region leakage components in orthogonal or triangular geometries. Overhead is minimized by requiring only one I/O pass over the unnormalized flux data. Depending opon the requested edit options one or more sweeps across the resident block of fluxes may be required. In the first sweep, fluxes are

power-normalized, written and optionally editted. The group-integrated fluxes by mesh cell are accumulated also. In adjoint problems an additional I/O pass is required to reverse the flux group ordering for integral edits. An additional NBLKR sweeps (NBLKR is the number of region blocks) over the resident block of flux planes are made to compute the region flux integrals and the leakage component integrals for the neutron balance edits. Prior to exiting SSTOU2 the region-to-mesh-interval map is converted back to a zone-to-mesh-interval map.

The DSSTO3 overlay optionally calls three subroutines (BALINT, FLXINT and FLXRZ) which edit the region and area balance integrals, the region and area flux integral totals and/or the region averaged fluxes, and the zone-averaged fluxes (e.g. the kZFLUX file), respectively.

4.1.11 SUMMARY (ANL only)

The SUMMARY module is used with DIF3D at ANL to edit summary reaction rates and isotopic masses. It is evoked whenever the A.SUMMAR data set is supplied with the input data (the single card-image "DATASET=A.SUMMAR" is sufficient data to trigger a SUMMARY edit). The interface files RTFLUX, GEODST, ISOTXS, NDXSRF, ZNATDN and COMPXS must also be present (these normally exist following a typical DIF3D calculation). If present, SUMMARY will also use the LABELS, PKEDIT, and NHFLUX files.

4.1.12 UDOIT1-UDOIT4

The four UDOIT modules, UDOIT1 - UDOIT4 are user modules placed at strategic points in D3DRIV to provide the user with additional processing capability during the calculational sequence (see Fig. 1.1). This feature of DIF3D is particularly useful in modular systems where the dummy UDOIT modules may be easily pre-empted by user UDOIT modules located in an automatic-call library that may be processed via the ARCSP021 procedure parameter PRELIB='name'. The user merely creates a self-contained load module which communicates with the DIF3D system via the appropriate interface files and thereby tailors DIF3D processing capabilities to suit his needs. This feature may be exploited in stand-alone implementations by relinking DIF3D with dummy user overlays appropriately replaced. Four interface file names (three binary files UDOIT versions 1, 2 and 3 and one BCD file A.UDOIT) are reserved in the SEEK file table for UDOIT applications.

4.2 Data Set Classification and Use by Code Block

Table 4.1 lists all of the data sets used by the code blocks in DIF3D and classifies them into one of five different categories:

BCD: Formatted, sequential access input and output, including standard system data sets (see definitions in Appendix B);

CDB: Code-dependent (including ARC system) binary (unformatted sequential access) interface data sets (see definitions in Appendix D);

CCCC: CCCC binary interface data sets (see definitions in Appendix C);

DOPC: Unformatted random access scratch data sets;

SCR: Sequential access scratch data sets.

TABLE 4.1. Data Set Classification and Description

File Reference Number	File Name	File Type	File Description
4	DSPLASC1	SCR	graphics scratch file
5		BCD	input data for SCAN module
6		BCD	output data all modules
8	DSPLAFNT	CDB	graphics font data
9		BCD	input data spool from SCAN
10		BCD	auxiliary output all modules
11	A.DIF3D	BCD	DIF3D control
12	A.NIP3	BCD	GNIP4C control
13	A.HMG4C	BCD	HMG4C control
14	A.LASIP3	BCD	LASIP3 control
15	A.ISO	BCD	BCD ISOTXS
16	BCDSOB	BCD	BCD LASIP3 output
17	A.SUMMAR	BCD	SUMMARY control
18	DIF3D	CDB	DIF3D control
19	COMPXS	CDB	macroscopic cross sections
20	LABELS	CDB	labels, half-heights
22	D3EDIT	CDB	tabular edits spool
23	NHFLUX	CDB	nodal restart (real)
24	NAFLUX	CDB	nodal restart (adjoint)
25	PKEDIT	CDB	peak power/flux interface
26	GEODST	CCCC	geometry description
27	ISOTXS	CCCC	microscopic cross sections
28	NDXSRF	CCCC	nuclide/zone reference
29	ZNATDN	CCCC	zone nuclide atom densities
30	RTFLUX	CCCC	real flux
31	ATFLUX	CCCC	adjoint flux
32	FIXSRC	CCCC	fixed source
33	RZFLUX	CCCC	zone flux averages
34	PWDINT	CCCC	power density
35	ISNTXS	CCCC	aux. ISOTXS slot
36	ISOTX1	CCCC	aux. ISOTXS slot
37	ISOTX2	CCCC	aux. ISOTXS slot
38	SNCONS	CCCC	S_n constants (transport)
39	SEARCH	CCCC	SRCH4C control
41-56	RNDMnn	DOPC	random access scratch files (Table 4.3)
61,62	XSISO	CDB	micro. cross section files 1 and 2
66-75	SCR001-10	SCR	scratch files
76-78	UDOIT	CDB	UDOIT versions 1-3
80	AUDOIT	BCD	UDOIT module input

The file reference numbers are assigned in the SEEK initialization call. In the Argonne implementation of the CCCC routines REED/RITE and SEEK, the Fortran logical unit numbers are identical to the file reference number. The absence of a file name in Table 4.1 indicates a system data set; these do not appear in the SEEK table. Files of type DOPC are listed in Table 4.3 (Section 4.3). The Argonne implementation of DOPC (see Sections 4.3.4.3 and 4.3.4.1) assigns Fortran logical unit numbers to DOPC files RNDM01 - RNDM14 via a call to SEEK. This, of course, has no effect on other DOPC implementations (i.e., the data set names RNDM01-RNDM14 will never be referenced). The data sets accessed by a given module are summarized in Table 4.2.

TABLE 4.2. Interface File Usage by Module

Module	Input Files	Output Files
SCAN	BLOCK=OLD and BLOCK=dsname (BCD card image input)	ARCBCD (BCD input data spool
STUFF	BLOCK=STP021	BCD input files from BLOCK=STP021
UDOIT1,2,3,4	See footnote a	See footnote a
CSE010	XS.ISO or ISOTX1, ISOTX2	ISOTXS (on ISNTXS unit)
LASIP3	A.LASIP3 and CCCC interface files	CCCC interface files
GNIP4C	A.ISO, A.NIP3, GEODST, NDXSRF, ZNATDN, ISOTXS, FIXSRC, SEARCH	ISOTXS from A.ISO, GEODST, NDXSRF, ZNATDN, FIXSRC, LABELS, SEARCH from A.NIP3
HMG4C	A.HMG4C, A.NIP3, LABELS, ISOTXS, NDXSRF, ZNATDN	COMPXS
MODCXS	A.NIP3, COMPXS, LABELS	COMPXS
BCDINP	A.DIF3D, DIF3D	DIF3D
SRCH4C	SEARCH, RTFLUX or DIF3D, NDXSRF,ZNATDN, GEODST, LABELS	SEARCH, NDXSRF, GEODST, LABELS
DIF3D	DIF3D, GEODST, COMPXS, FIXSRC, LABELS, RTFLUX, ATFLUX, SEARCH, SNCONS, UHFLUX, NAFLUX	DIF3D, RTFLUX, ATFLUX, RZFLUX, PWDINT, D3EDIT, PKEDIT, NHFLUX, NAFLUX
SUMMARY	A.SUMMAR, GEODST, COMPXS, ISOTXS, NDXSRF, ZNATDN, RTFLUX, NHFLUX, PKEDIT, LABELS	

[a]Files A.UDOIT and UDOIT (versions 1, 2 and 3) are available in the SEEK table and intended for UDOIT module applications.

4.3 Data Management Considerations

A multilevel transfer approach that unifies the treatment of one- or two-level storage hierarchy machines is adopted in DIF3D. The implementation employs a set of high level subroutines to perform the data management tasks. These subroutines in turn exclusively employ the standardized utility subroutine calling sequences defined by the CCCC[6], thereby providing a highly exportable code system that has been tailored to utilize machine-dependent multilevel and random access I/O methods.

4.3.1 Data Management Concepts

The following terminology will be used in the ensuing discussion (see Ref. 6 for more detailed definitions):

1. Extended Core Memory (ECM): That (physically separate or logically designated) portion of a computing system containing storage locations which serve as a buffer for random access data.

2. ECM File: A named array allocated within the BPOINTER ECM container. This array provides a buffer area for one or more blocks of random access file data. Associated with an ECM file is a block structure identical to the random access files it services.

3. Fast Core Memory (FCM): That portion of a computing system which contains storage for both data and instructions, which is directly coupled to the computations portion of the system, and which is directly coupled to ECM. FCM may be the entire central memory or it may be that portion of central memory remaining after an ECM portion is designated.

4. Random Access Data: Data which can be transferred between FCM and ECM in out-of-sequence strings.

5. String: A subportion of a random access file block. Data transfers beween FCM and ECM are string transfers.

6. Random Access File: (Also called Direct Access File). A named collection of data which is stored on a peripheral storage device. The file data are arranged in blocks which can be transferred between ECM and peripheral storage randomly, i.e. out of sequence.

7. Logical File: A random access file. The identity of a logical file in DIF3D is established by an integer variable, the (logical) file reference (or unit) number.

8. Logical Record: A basic unit of information used in the definition of a logical file; all records in a logical file are the same length.

9. Logical Record Group: A logical collection of records. Each record group in a file has the same number of records (e.g. a group and space-dependent flux file has each flux plane of each group as a record and all flux planes (records) in a particular energy group as a logical record group).

10. Block: A collection of logical records in a record group of a random access file. Each block consists of an equal number of records (N) except for the last block in a record group which may have M<N records. The block length is always less than or equal to the record group length. Data transfers between disk and ECM are block transfers.

11. Disk: A generic name for a peripheral storage device used for storing random access files.

12. Physical Unit: An identifiable subpart of a disk. One of more physical units comprise a disk.

13. File-Group: A collection of one or more random access files. The file-group collection is assigned to a single physical unit.

4.3.2 Multilevel Data Management Strategy

The standardized method[6] of multilevel data management employs the data transfer paths illustrated in Fig. 4.5. Each random access file is composed of one or more record groups and resides on a physical unit. When needed, data is transferred (via DRED and DRIT) in blocks of records between disk and ECM, and then strings of data are transferred (via CRED and CRIT) between ECM and FCM. When the ECM and FCM BPOINTER containers both reside in the same memory level, data from ECM is used directly, thereby avoiding redundant memory allocation and data transfer. Most of the bookkeeping associated with this data management approach is consolidated and eliminated by the high level data management routines described in Section 4.3.4.

The principal goal of the DIF3D data management strategy is to minimize the use of costly random access I/O transfers by optimizing the use of the available ECM container (ECM size is specified on the type 02 card of A.DIF3D). As mentioned in Section 3.9.1 two principal strategy options, the one-group-contained option and the concurrent inner iteration option, are available to achieve this goal. The latter option performs one or more I/O sweeps across the data required in the within-group (inner) iteration for a given outer iteration because the data for all planes in the current group are not simultaneously contained in ECM. The former option requires exactly one I/O pass across the data. As ECM size is increased beyond the one-group-contained threshold an attempt is made to contain additional data, namely, a scattering band of fluxes or the entire flux file, and/or cross sections, finite-difference coefficients and fission sources. Ultimately, a third option, all files ECM-contained, is possible at which point no DOPC files are required except for the DOPC file FSRC in inhomogeneous source problem.

The principal data structures in the strategy options are the ECM files through which all data are buffered for the (up to 14) random access disk files listed in Table 4.3. The block structure of an ECM file is identical to the structure of the random access disk files that it will service. However, only a subset of the total number of blocks in a DOPC file is typically allocated to an ECM file in most strategy options.

Data is transferred between the random access scratch files in Table 4.3 and the corresponding ECM files listed in Table 4.4 using the DIF3D data management routines BLKGET and BLKPUT which in turn call the standardized CCCC[6]

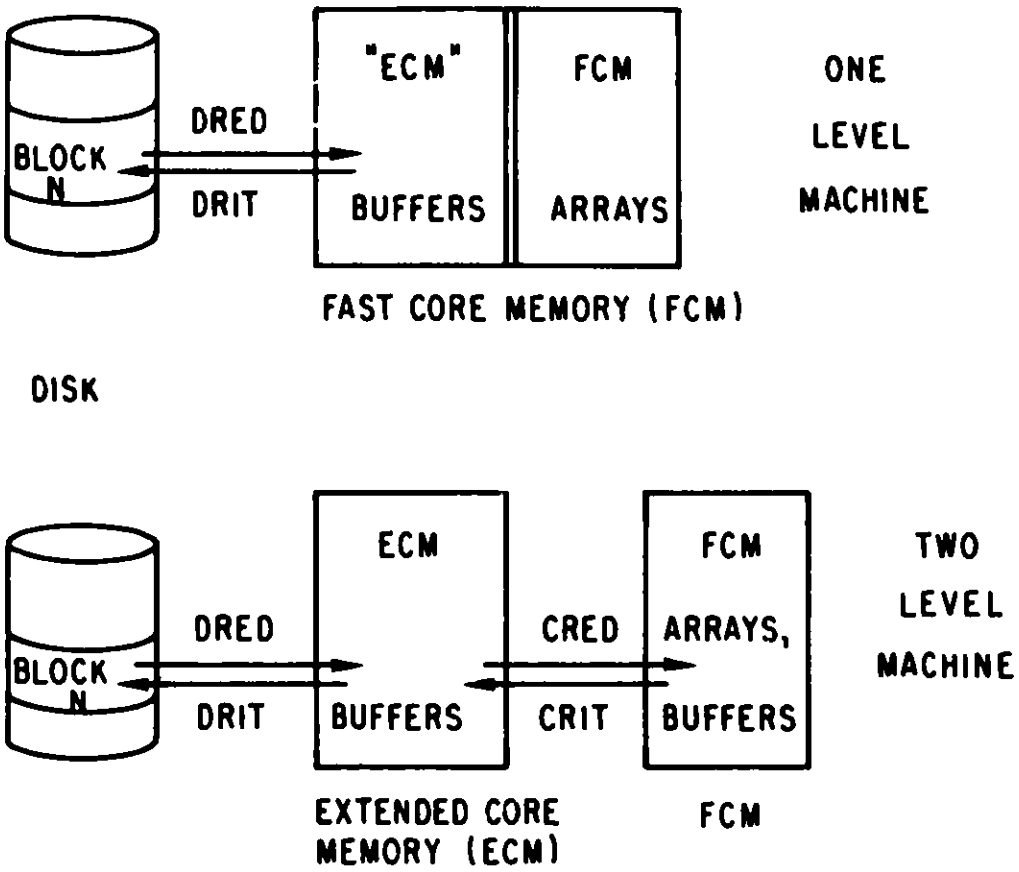

Fig. 4.5. Multilevel Data Transfer Paths

TABLE 4.3. Random Access File Descriptions

DOPC Reference Number	File Group Number	SEEK Reference Number	SEEK Table File Name	ARCSP021 File Name
1	2	41	RNDM01	PSIOLD
2	3	42	RNDM02	PSINEW
3	5	43	RNDM03	PSIUP
4	1	45	RNDM04	FDCOEF
5	2	46	RNDM05	FRNOLD
6	3	47	RNDM06	FRNNEW
7	4	48	RNDM07	FRNM1
8	5	49	RNDM08	FRNM2
9	4	51	RNDM09	SRCNEW
10	1	52	RNDM10	ZONMAP
11	6	53	RNDM11	CXSECT
12	4	54	RNDM12	FSRC
13	2	55	RNDM13	PSIGO
14	3	56	RNDM14	PSIGN

TABLE 4.4. Correspondence Between ECM and Disk Files

ECM File Name	Disk File Name	File Contents
ZONMAP	ZONMAP	Zone to fine mesh map
CXSECT	CXSECT	Macroscopic cross sections
ZONMPC*	--	Zone to coarse mesh cell map
PSINEW	PSIOLD,PSINEW	Flux iterate (all groups)
BPSI*	PSIGO**,PSIGN**	Flux iterate (current group)
FDCOEF	FDCOEF	Finite difference coefficients
SRCNEW	SRCNEW**	Group total source
FRBUFS	FRNM1,FRNM2	Fission source iterates
FRNM1**,2**	FRNOLD**,FRNNEW**	
CXSADJ	CXSECT	Adjoint ordered cross sections
VOLUME	--	Unit height mesh cell volumes in X-Y plane
AREATC*	--	Cross sectional area for any X-Y plane
AREAFC*	--	Cross sectional area for any X-Z plane
AREALC*	--	Cross sectional area for any Y-Z plane
REGMPC	--	Region to coarse mesh cell map
POWERF	PSIGO**,PSIGN**	Power density by mesh cell
PEAKFL	FRNNEW**	Peak total flux by mesh cell
PEAKFF	FRNOLD**	Peak fast flux by mesh cell
PEAKPW	SRCNEW**	Peak power density by mesh cell
SRFBUF	SCR001,2	Surface fluxes by mesh cell
RPWINT	SCR001	Region power integrals
APWINT	SCR002	Area power integrals
TOTPSI	PSIGO**,PSIGN**	Total flux by mesh cell
RPSINT	SCR001	Region flux integrals
APSINT	--	Area flux integrals
RBLBUF	SCR006,3,4	Region balance (leakage) integrals
RBLINT	SCR003,1,2	Region balance integrals
RBLTNT	SCR003,1,2	Region balance integral totals
ABLINT	SCR004,5	Area balance integrals
ABLTNT	SCR004,5	Area balance integral totals
ZPSINT	SCR005	Zone-averaged flux integrals

* Temporary ECM files
** CIIS option only

routines DRED and DRIT. ECM files are opened (via calls to OPENCF) with the number of blocks required by the current data management option.

Except for ZONMAP and CXSECT which are defined in SSINIT, all ECM files in the upper half of Table 4.4 are defined (via DEFICF) in subroutine SSTATE. ECM files in the lower half of Table 4.4 are defined in one of the three edit overlay drivers (DSST01, DSST02 or DSST03). The ECM files are not opened (i.e. ECM container space is not suballocated to a particular ECM file) until an OPENCF call is issued. When an ECM file is no longer needed its ECM space may be via a call to CLOSCF. The definitions of the DOPC files are made (via DOPC and DEFIDF) in subroutine SSDISK. The characteristics of the ECM and DOPC files are provided in the subroutine calls to DEFICF and DEFIDF and will not be repeated here.

Several of the ECM files in Table 4.4 are temporary files needed during preliminary stages of the DIF3D calculation (e.g. ZONMPC, CXSADJ, AREATC, AREAFC and AREALC). The temporary files use ECM space that will later be reused by the major ECM files during the outer iteration strategy.

Numerous small arrays are allocated in the FCM container. Documentation of these arrays occurs in the source listings of the subroutines which use them. Data transfer required for these arrays is performed by the CCCC routines REED and RITE. An auxiliary group of arrays are allocated in FCM on two-level machines, of which the CDC 7600 is the only machine on which we have had operating experience. These FCM arrays provide a computational buffer area in which data passed from ECM may be efficiently processed, thereby avoiding the less efficient computations that result when ECM files are directly addressed (see discussion in Section 4.3.2.3).

The auxiliary edit files in the lower half of Table 4.4 are opened at different stages in the editing overlays. A number of these ECM files are region and area integral files which have a logical record group structure similar to the flux files. Within a record group, however, blocking is simply based on the available ECM container space; a natural block size (such as a mesh plane in files of mesh cell data) does not exist. Because of the special nature of these region and area files and their relatively limited resource utilization, the BLKGET and BLKPUT routines are not used to transfer data between disk and ECM. Instead we use the sequential access routines REED and RITE to transfer data from scratch files SCR001-SCR006 directly to ECM files on one-level machines. On two-level machines auxiliary FCM sub-blocks are allocated for computational efficiency (as noted in Section 4.3.2.3) and data is transferred between disk and FCM using REED and RITE. After processing a sub-block of data pertinent sub-blocks are transferred between FCM and ECM using CRED and CRIT. Several sub-blocks of data may then be successively saved in and reused from ECM until the next region or area block is required.

4.3.2.1 The One-Group-Contained Strategy

In this strategy each block of an ECM file contains all data for at least one energy group (i.e. all mesh planes in mesh cell dependent files). Therefore, each ECM file requires one block of appropriate size. During the outer iterations the FDCOEF and BPSI files are alternately opened and closed once each outer to permit the reuse of ECM space. When a scattering band of fluxes is ECM-contained, the ECM file (PSINEW) is opened with MAXSCT+1 blocks

where MAXSCT is the maximum scattering bandwidth. The BPSI file is not used in this case. The three most recent iterates of the fission source file are required for the Chebyshev acceleration of the outers. The two most recent iterates are held in the ECM file FRBUFS which unlike the other ECM files is normally assigned two blocks. The oldest iterate is buffered through the ECM file SRCNEW alternately from DOPC files FRNM1 or FRNM2 on which it had been previously saved. When sufficient ECM space exists, three blocks are allocated to FRBUFS thereby permitting the three most recent fission source estimates to ECM contained.

4.3.2.2 Concurrent Inner Iteration Strategy

The concurrent inner iteration strategy (CIIS) requires that data for only a fraction of the total number of mesh planes be ECM-contained during the within-group inner iterations. Consequently, three-dimensional problems with an unlimited number of mesh planes are permitted with the number of mesh cells on a plane dictated by the ECM container size.

The K planes in each energy group are partitioned into Q blocks of planes with block size L. An upper bound on the block size L is an input parameter on the type 03 card of A.DIF3D. This bound represents an estimated optimal block length for efficient I/O performance on a particular machine. As mentioned in section 3.10.1, an attempt is made to ECM contain as many blocks of planes of size L as is possible with the given ECM container size.

The CIIS algorithm is sketched in a FORTRAN-like notation in Fig. 4.6.

The inner iterations sweep across the mesh planes in a wave-front fashion, processing all data on a particular plane before proceeding to the next plane. As an inner iteration for one block completes, the next iteration for all preceding blocks can be performed. U, the effective number of blocks which can be simultaneously contained in ECM determines the wavefront or bandwidth of inner iterations (B=UL) which can be performed in a single I/O pass over the current group data. After the B'-th iteration has completed for all planes in a given block the write operation for the block may be initiated. Although the calculations for the new flux in this block are completed, the block must remain in ECM for the next I/O cycle because data in the last plane of the block is required during the next cycle. During this cycle the asynchronous write operation is given time to complete. The number of inner iterations, M_g, for each outer iteration determines the number of I/O passes, P_g,

$$P_g = (M_g + B - 1) / B$$

required to complete the inner iterations in group g. A diagram of the I/O and CPU activity that occurs in the ECM file PSINEW on two successive I/O cycles c and c+1 is illustrated in Fig. 4.7.

In summary, each inner iteration pass, p=1,2,...,P_g, is comprised of c=1,2,...,C I/O cycles. The following events occur in cycle c:

1. The asynchronous reads for block c (c<Q) are completed and reads for block c+1 (c<Q) are initiated.

2. In the first pass (p=1) the group source for block c is calculated and saved for for later passes.

```
      Q = (K+L-1) / L
      B = U * L
      C = U+Q
      DO 400 g = 1,NGROUP
         P_g = (M_g-1)/B + 1
         DO 300 p = 1,P_g
            B' = min( B, M_g-(p-1)*B )
            'initiate reads on block (1,g) data'
            DO 200 c = 1,C
               IF (c≤Q) 'finish reads on block (c,g) data'
               IF (c<Q) 'initiate reads on block (c+1,g) data'
               IF (c≤Q and p=1) 'calculate block (c,g) group source'
               DO 100 b = 1,B'
                 K_s = max( 1, c*L - b - L + 1 )
                 K_e = min( K, c*L - b )
                 IF ( K_s≤K_e ) 'perform inner iteration for planes K_s to K_e'
100            CONTINUE
               IF (c>U+L) 'finish write of flux block (c-U-1,g)'
               IF (c>U) 'initiate write of flux block (c-U,g)'
               IF (p=P_g and c>U) 'compute fission source for block (c-U,g)'
               IF (p=P_g and c>U and g=G) 'perform Chebyshev acceleration on
                                           fission source block (c-U,g)'
200         CONTINUE
            'finish writes on flux block (Q,g)'
300      CONTINUE
400   CONTINUE
```

Fig. 4.6. Concurrent Inner Iteration Algorithm

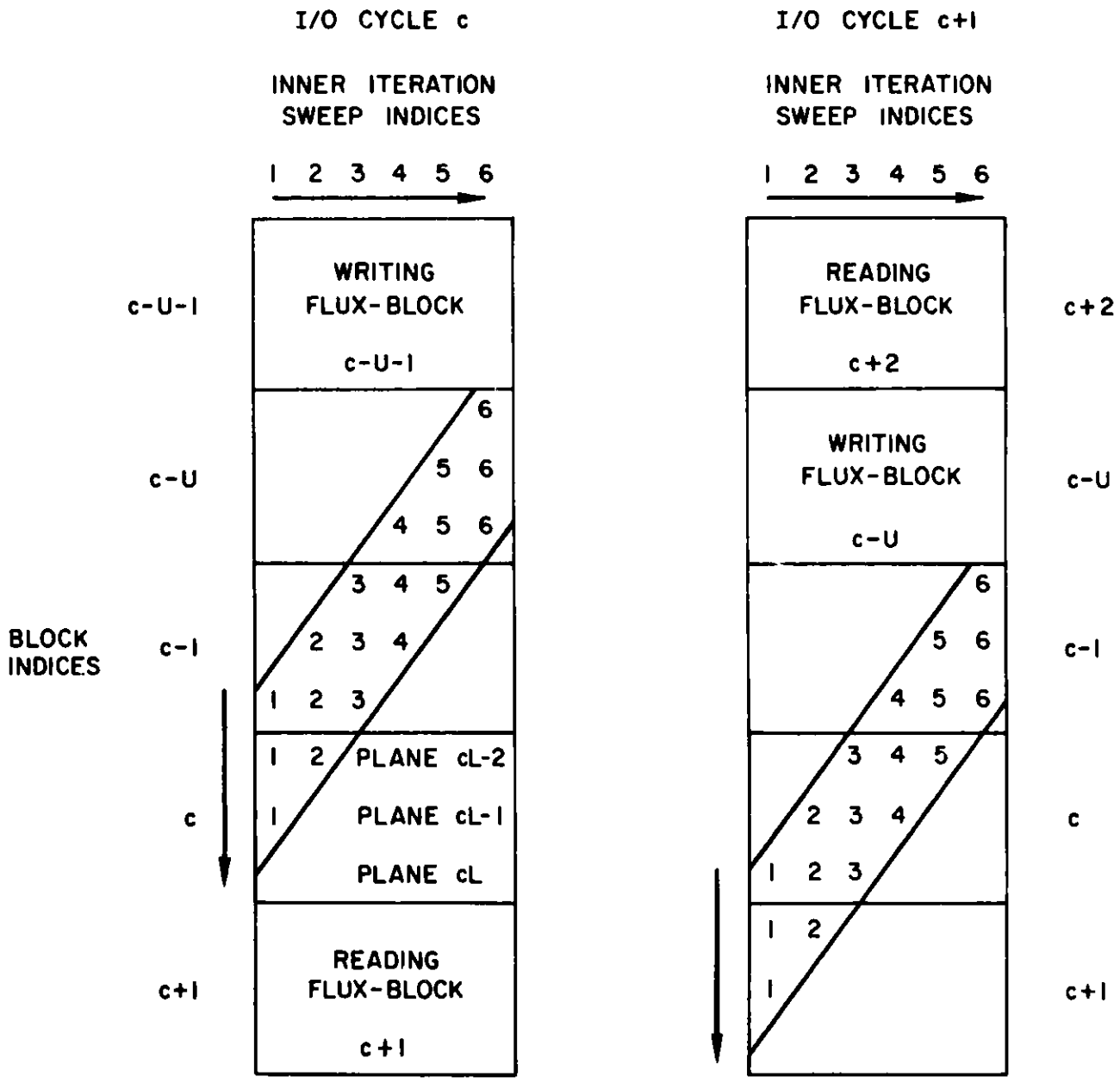

Fig. 4.7. Concurrent Inner Iteration I/O Cycle Description (L=3, U=2)

3. The B' inner iterations for blocks c-U to c are performed (See Fig. 4.7).

4. The write for flux block c-U-1 is completed and the write for block c-U is initiated.

5. On the last pass P_g the block c-U fission source is calculated and Chebyshev acceleration is applied.

The storage requirements (in units of mesh planes) for the variable size CIIS blocks are summarized by:

1. U+3 fluxes,

2. 4(U+2) finite difference coefficients,

3. U+2 total group sources,

4. 4+1/LDW miscellaneous data (3 fission sources, 1 flux and 1/LDW zone map).

The constant terms in these storage requirements formulas account for auxiliary blocks required to achieve a high degree of I/O and CPU concurrency. LDW is a word length parameter which accounts for the fact that integer array storage requirements are half that of long words on short word machines. The procedure for estimating the optimal ECM size for a given problem and for determining the appropriate value for U is presented in Section 3.10.1.

4.3.2.3 Two-Level Machine Data Management Considerations

As mentioned earlier (Section 4.3.2) transfers between ECM files and FCM arrays use the CCCC utility routines, CRED and CRIT. This practice avoids the inefficiencies obtained when single data items are directly addressed at random locations in ECM. After allocating required fixed size arrays in FCM including the cross sections array for one group, the remaining plane-oriented mesh cell arrays are blocked with one or more mesh lines per block based on the FCM container size (specified on card 02 of A.DIF3D file).

Because of the regular nature of the mesh cell structure in the DIF3D finite difference option, the two-level strategy is implemented with no essential change to the solution algorithm. Loops over the J lines in a plane are replaced by an equivalent set of two loops; a loop over blocks of lines in a plane and a loop over lines within each such block. The one-level implementation simply uses the special case of all J lines contained in a single block.

Prior to processing each block of lines, data from appropriate ECM files must be transferred to FCM (via CRED). After processing each block of lines newly calculated data must be transferred to ECM (via CRIT). The pointers to the FCM arrays used which receive the ECM data are always passed as subroutine arguments to the routines in which the CRED and CRIT occur. On one-level implementations these pointers are set to the appropriate location in the directly addressable ECM file.

Coding which is pertinent only to the two-level data transfers (e.g. CRED and CRIT calls and associated indexing) is bracketted by C2LV comment cards[41] which are "activated" by a preprocessor code when generating a two-level implementation of DIF3D. When partial plane blocking is required in FCM, additional coding is required for initialization tasks in the next-adjacent-face periodic boundary condition option. An additional array is needed to contain the boundary fluxes (along the lower X-boundary on plane k) which are required in the transverse leakage calculations for the j=1 line on plane k. A similar array is needed for the reverse calculation.

4.3.3 DIF3D Data Management Routines

The high level data management routines developed for DIF3D are designed to simplify the bookkeeping associated with managing the disk and ECM files in a variety of machine environments. These routines employ the BPOINTER routines[41] to manage ECM file allocations in the ECM container and call the CCCC routines DOPC, DRED and DRIT to perform asynchronous, random access I/O tasks.

The DIF3D routines may be logically divided into two primary groups, those related to ECM files and those related to DOPC files. The first group includes DEFICF, OPENCF, CLOSCF, PURGCF, ENTGET and PCRED. They communicate with each other via the CFTABL COMMON block in which is located data defining the characteristics and current state of each ECM file. The second group includes DEFIDF, OPENDF and CLOSDF which communicate via the RNDMFL COMMON block in which is located data defining the characteristics and current state of each DOPC file. The BLKGET subroutine with entry points (FINGET, BLKPUT and FINPUT) controls data transfer between DOPC files and ECM files and therefore belongs to both groups.

The PCRED routine with entry points (ICRED, PCRIT and ICRIT) is a recent addition to these data management routines and is employed only in the nodal option.

4.3.3.1 DEFICF

The characteristics of each ECM file are specified to the DIF3D data management routines by a call to DEFICF. The calling sequence for DEFICF is:

```
CALL DEFICF ( CFNAM, NREC, LREC, NRBLK, NRGRP, LCFN)
```

This call defines the characteristics of ECM file, CFNAM, which has NREC records of length LREC (single precision) words. There are NRBLK records in a block and NRGRP records in a record group. LCFN is the ECM file reference number by which this file may be addressed and is simply the index of the next available entry in the ECM file table in COMMON block CFTABL. Calling DEFICF with CFNAM = CLEARC will initialize the CFTABL COMMON block.

Entry point DELECF deletes file CFNAM and zeroes its CFTABL entries. Entry point CHNGCF changes the name of the ECM file having reference number LCFN to the name CFNAM.

4.3.3.2 OPENCF

After the characteristics of an ECM file have been defined (via DEFICF), ECM container space may be suballocated for it via a call to OPENCF:

```
CALL OPENCF( CFNAM, LCFN, NBUFS, IFTYP )
```

This call issues a call to the BPOINTER routine PUTB to allocate an array named CFNAM. The call allocates space for NBUFS blocks where the size of a block was given in the DEFICF call. The sentinel IFTYP signals one of two operational modes for the ECM file. Files that require I/O transfers are designated with IFTYP=1. Random access files that are ECM-contained and require no I/O transfers are designated by IFTYP=0. Subsequent calls to BLKGET or BLKPUT will automatically ignore I/O requests for these files. Note below the effect of CLOSCF calls with action sentinel unity on IFTYP=0 files.

Calls to OPENCF for files that have already been opened are ignored if either the file is already ECM-contained or if the existing file is not ECM-contained but has sufficient space to contain the requested NBUFS blocks. A file opened with IFTYP=1 can be changed to ECM-contained mode (IFTYP=0) by calling OPENCF with IFTYP=0 provided NBUFS is identical to the existing number of blocks already allocated.

4.3.3.3 CLOSCF

When an ECM file is temporarily or permanently no longer needed, the CLOSCF subroutine may be used to release the buffer space. The calling sequence for CLOSCF is:

```
CALL CLOSCF ( LCFN, NOP )
```

This call releases the suballocated buffer space for the ECM file with reference number LCFN depending on its associated OPENCF sentinel and the action sentinel NOP. If NOP = 0 or 2, the buffer space is unconditionally released (via the BPOINTER WIPOUT command). When NOP = 0 this call also deletes (via an internal DELECF call) the ECM file from the list of files in the CFTABL common block. Calls to CLOSCF with NOP = 1 are ignored when the file is ECM-contained (i.e. opened with IFTYP = 0).

4.3.3.4 PURGCF

Following one or more calls to CLOSCF, the released ECM container storage may be recycled for subsequent use by calling PURGCF. The calling sequence for PURGCF is:

```
CALL PURGCF (LSTBUF)
```

PURGCF calls the BPOINTER routine PURGEB to clean up a fragmented ECM container and then refreshes the ECM pointers for all ECM files that remain open. A pointer to the first unused ECM location is returned in LSTBUF.

4.3.3.5 BLKGET, FINGET, BLKPUT and FINPUT

All I/O requests to random access files are channeled through BLKGET and FINGET or BLKPUT and FINPUT which ultimately invoke the CCCC routines DRED or DRIT. The calling sequence for BLKGET (which calls DRED) is:

```
CALL BLKGET ( LCFN, NCBLOK, LDFN, NDBLOK )
```

This call requests the NDBLOK-th block from the random access file with DOPC reference number LDFN to be read into the NCBLOK-th block of the ECM file having reference number LCFN. A corresponding FINGET call is required to ensure that the potentially asynchronous I/O operation has completed prior to using the requested data. An identical calling sequence is required for the BLKPUT and FINPUT routines for writing random access files to disk.

If the designated ECM file is core-contained (IFTYP=0 in the OPENCF call) no data transfer requests are issued by these routines. If NBUFS denotes the number of blocks allocated to an ECM file, then the block in which the data transfer occurs is determined as NCBLOK modulo NBUFS. This enables the programmer to use the natural block index of the DOPC file rather than the index imposed by the size of the ECM file. In most applications NCBLOK and NDBLOK will be identical.

4.3.3.6 DEFIDF

Members of DOPC random access file groups are defined via calls to DEFIDF. The calling sequence of DEFIDF is:

```
CALL DEFIDF ( DFNAME, LDFN, MXBLOK, MXLEN, LENFIL )
```

This call defines the characteristics of the random access file having DOPC reference number LDFN. The maximum number of blocks (MXBLOK), the maximum block length (MXLEN) and the length of the file (LENFIL) are the parameters passed on to DOPC within DEFIDF. The file name DFNAME is used internally by the DIF3D data management routines for the programmer's convenience.

The random access file table in the RNDMFL COMMON block must be initialized by calling DEFIDF with file name CLEARD prior to defining the first DOPC file. A DOPC initialization call (action code 0) will also be made by DEFIDF. A DOPC file group is defined by calling DOPC with action code 3 following one or more DEFIDF calls which define the member files of the corresponding file group. Null files are defined when MXBLOK=0 and provide a means for simplifying program logic. Such files are not added to DOPC file groups, but are entered into the random file table COMMON block, RNDMFL.

4.3.3.7 OPENDF and CLOSDF

The calling sequence for OPENDF is:

```
CALL OPENDF ( DFNAME, LDFN )
```

This call returns the DOPC reference number (LDFN) associated with a random access file name and does not initiate I/O activity.

The calling sequence for CLOSDF is:

```
CALL CLOSDF ( LDFN, NOP )
```

This call closes the random access file with DOPC reference number LDFN by calling either DRED or DRIT with record number zero. The choice of DRED or DRIT depends on the most recent file activity. When action flag NOP = 0, the associated file is deleted from the random access file table.

4.3.3.8 PNTGET and IPTGET

Pointers to particular records within an ECM file are obtained by subroutine PNTGET. The calling sequence for PNTGET is:

```
CALL PNTGET ( LCFN, ICREC, LPT )
```

This call returns the pointer (LPT) to record number ICREC in the ECM file denoted by the reference number LCFN. LPT is a pointer relative to a long word ECM container array. A long word array is single precision on a long word computer such as the CDC 7600 or the CRAY-1. On short word machines (e.g. IBM 3033) a long word array is a double precision (REAL*8) array. A similar calling sequence used with IPTGET returns the pointer (LPT) to a requested record in the LCFN file relative to a short word (single precision) ECM container array.

On two-level implementations the ECM container is never directly addressed therefore PNTGET is made equivalent to IPTGET. The pointers are then appropriate for use in the CRED/CRIT routines which transfer data between ECM and FCM.

4.3.3.9 PCRED, ICRED, PCRIT and ICRIT

PCRED and ICRED combine the functions of returning ECM pointers to a requested record of an ECM file (a PNTGET or IPTGET function, respectively) and then, on two-level machines, transferring data for the requested record from ECM to FCM (a CRED function). The calling sequence for PCRED is:

```
CALL PCRED ( NCFN, ICREC, MCPNT, LCPNT, NREC, IREAD )
```

This call returns the pointer (MCPNT) to record number ICREC in ECM file NCFN. In one-level machine implementations the ECM container is directly addressable, therefore PCRED also sets the FCM pointer LCPNT to MCPNT prior to return. In two-level implementations LCPNT is an input argument to the PCRED call and NREC records are transferred to FCM (starting at FCM pointer LCPNT) from ECM file NCFN (starting at ECM pointer MCPNT) whenever the sentinel IREAD is nonzero.

In two-level implementations PCRIT and ICRIT transfer NRECS records from FCM (starting from FCM pointer LCPNT) to ECM file NCFN (starting from ECM pointer MCPNT). MCPNT must be already defined before a PCRIT or ICRIT call is made.

4.3.3.10 STATCF

STATCF is a debugging tool that displays the currently defined ECM files and their associated characteristics.

4.3.4 CCCC Utility Routines

Reference 6 describes a set of subroutine calls defined by the Committee on Computer Code Coordination (CCCC) which standardizes data management in order to facilitate the exchange of programs between different computers and laboratories. Only the calling sequences and functions are standardized; the actual coding of each routine is left to individual installations.

The set of routines[41] developed at ANL are designed to operate on machines with either one level of memory (e.g. IBM and Cray computers) or two levels (e.g. the CDC 7600). The machine-dependent coding has been kept to a minumum. Not only does this approach make code export easier, it also permits the testing of a two-level data-management strategy on a one-level machine.

The calling sequences and functions are defined fully in Ref. 6. This section goes into some of the coding details for the versions of the CCCC subroutines included in the utility subroutine package.

4.3.4.1 SEEK

In the ANL implementation of the CCCC standards all data sets except the output print file and input card image file are given names and version numbers. Some file formats (e.g. those containing isotopic neutron cross sections or the neutron flux distributions) are defined by the CCCC, but others (e.g. the file used by Applied Physics codes to store macroscopic cross sections) are code-dependent. Subroutine SEEK provides the connection between file names and logical unit numbers, even for scratch files. SEEK is very similar to the ARC System routine SNIFF[36].

SEEK must create and maintain a table (the "SEEK table") that associates each unique file name and version number pair with a "file reference number". The SEEK table must also tell whether a file "exists" (i.e. has had something written into it) or not. The method of initializing the SEEK table is entirely up to the individual installation. The ANL version of SEEK permits two different methods for initialization. Both are described in the writeup of SEEK in Appendix A of Reference 41. One is the same as the procedure required by SNIFF, the other is more flexible. SEEK must be initialized before any files (binary or BCD) are read.

A distinction must be made between the "file reference number" used in the arguments of CCCC routines and the "logical unit number" that a programmer codes into a Fortran I/O statement. In the Los Alamos implementation of the CCCC standards the two are not the same. The programmer need not be concerned with the difference when dealing with binary files since all I/O is performed through calls to CCCC routines; applications programs should contain no Fortran statements such as READ or WRITE for binary files. It is a common ANL practice, however, to employ a number of BCD input files and to manage them with SEEK. This means that ANL coding contains calls to SEEK which reference file reference numbers as well as Fortran I/O READs and WRITEs which reference logical unit numbers for such BCD files. The correspondence between the two numbers is managed by means of a subroutine, SEKPHL, which is described later.

Because we employ subroutine SEEK with BCD and random access files in addition to sequential access files, it is instructive to review the following guidelines to avoid potential portability problems.

1. A call to SEEK with the proper read/write mode flag must be issued prior to the first read or write to a data set and prior to the first read or write to a data set that has been rewound. This practice is necessary for compatibility with implementations that dynamically assign logical unit reference numbers upon each call to SEEK and dynamically release logical unit numbers after a data set rewind command is received. A call to the appropriate routine, REED or RITE, with a record number of zero rewinds the data set.

2. The logical unit number for BCD data sets must be obtained by calling subroutine SEKPHL following the call to SEEK. SEKPHL returns the logical unit number corresponding to the logical unit reference number returned by SEEK. SEKPHL must also be used to rewind and close BCD files. See the SEKPHL example in Section 4.1.2; also see Ref. 41.

3. A set of fifteen generic file names (RNDM01-RNDM15) have been reserved for random access I/O applications. In order to maintain portability, calls to SEEK for random access data sets are embedded within our version of DOPC and DRED/DRIT. Consequently, SEEK calls for random access files are not otherwise necessary and should never be coded by the programmer.

4. Successive calls to SEEK (with different read/write mode flags) without intervening rewinds must be avoided. Such situations may arise when SEEK is called in a read mode solely to determine file existence. If the file exists, but the programmer does not intend to read the file, then REED (for binary files) or SEKPHL (for BCD files) should be called to rewind it. Later, if the file is actually to be read, SEEK must be called again. The compatibility issues raised on point 1 (above) apply here as well.

The version of SEEK in the utility package performs no finalizing or wrap-up function (NOP=2). The other operations specified by the CCCC standard are all implemented (NOP = 0, 1, 3, 4, 5).

4.3.4.2 REED/RITE

The CCCC standards require that all binary I/O operations be executed through calls to standard subroutines, not through Fortran I/O statements coded into applications programs. This practice permits individual installations to take advantage of locally available, efficient access methods without recoding programs; all that is needed is a local set of CCCC standard I/O routines.

REED and RITE are the CCCC routines specified for binary sequential data transfer between fast core (FCM) and external data files (disk). The calling sequence for REED is:

```
CALL REED(NREF,IREC,ARRAY(I),NWDS,MODE)
```

This call transfers NWDS single-precision words from record number IREC of the sequential file with logical unit reference number NREF to the FCM locations starting at the address of ARRAY(I). A similar call to RITE performs the inverse operation. MODE is a sentinel that permits a programmer to code buffered I/O. When MODE=0 I/O operations are completed before the return from REED/RITE. When MODE=1 I/O operations are not necessarily completed before the return to the calling program; a subsequent call with MODE=2 is required to complete the outstanding I/O operation.

The ANL version of REED/RITE includes IBM assembler language code that provides optional special access methods. In addition to providing the standard sequential I/O capability of the Fortran language, this version of REED/RITE provides an asynchronous, random access I/O capability. The SIO

program (see Section 4.4.3.1) is used to obtain this capability. In short, SIO uses IBM BSAM macro instructions, along with internal tables and absolute track addressing, to process the I/O requests. SIO was originally written for the OS/MVT operating system as a more efficient and more convenient alternative to IBM Fortran Direct Access. The current version of the routine runs under both OS/MVT and OS/MVS. The record format for SIO files must have the undefined attribute (RECFM=U). Since each logical record requires at least one track of direct access storage, the use of the SIO access capability for short record transfers is not efficient.

Within the REED/RITE subroutine, the RECFM parameter of a file's JCL is interrogated by a call to the subroutine RECFM. If the file has an undefined attribute (RECFM=U) the code will use SIO access methods. Any other record format (e.g. VBS, VS, FB, etc.) is processed by standard Fortran sequential I/O. To perform the SIO data transfers, a subroutine SIO is invoked. This routine in turn invokes the subtask SIOSUB which actually performs the I/O operations. The MODE parameter which is passed to REED/RITE is used to determine whether transfer is returned to the calling routine before the I/O operation is complete. This facility, therefore, provides the user with the ability to overlap I/O and CPU operations or I/O operations on one file with those on another.

4.3.4.3 DOPC and DRED/DRIT

The CCCC standards require that all random access I/O operations be channeled through calls to standard subroutines, not through Fortran I/O statements coded into applications programs. Also specified is the fact that such data should be transferred between external data files (disk) and extended core memory (ECM).

The calling sequence for DRED is:

```
CALL DRED( NREF, IREC, LOCBFU, NWDS, MODE )
```

This call transfers NWDS single-precision words from record number IREC of the random access file with logical unit reference number NREF to the ECM locations starting LOCBFU words from the (user) ECM reference address (see IOP=0, below). A similar call to DRIT performs the inverse operations. MODE is a sentinel that permits the programmer to code asynchronous I/O. When MODE=0 operations are completed before return from DRED/DRIT. When MODE=1 I/O operations are not necessarily completed before return from DRED/DRIT; a subsequent call with MODE=2 completes the outstanding I/O operation.

Prior to calling DRED/DRIT the random access I/O implementation must be initialized by several DOPC calls. The five DOPC calling options are summarized below:

1. (IOP=0) Initialize DOPC and, in one-level implementations, supply a pseudo ECM reference location.

2. (IOP=1) Supply file characteristics for reference number NREF.

3. (IOP=2) Conclude the definition of the file group, NGREF. NGREF includes all files defined with IOP=1 calls since either the last IOP=2 call or the original IOP=0 call.

4. (IOP=3) Delete file group NGREF and its constituent files.

5. (IOP=4) Finalize DOPC at the conclusion of the program module. All file groups are deleted.

The connection between a random access file reference number NREF and its corresponding logical unit number is established in the ANL implementation by calling subroutine SEEK during the processing of each DOPC (IOP=1) call. The call to SEEK uses the generic random access file name RNDMnn which by convention corresponds to the random access file reference number NREF=nn. Currently NREF must satisfy 0<NREF<16. Codes which use this version of DOPC and DRED/DRIT need only supply in the SEEK initialization call those generic file names used by the applications code.

The DOPC initialization call establishes the pseudo ECM reference point for DRED and DRIT calls on one level machines. Although never explicitly specified in the CCCC standards, this pseudo ECM reference point initialization must also apply to CRED and CRIT usage. Consequently, all calls to DRED, DRIT, CRED and CRIT on one-level machines must be preceded by a DOPC initialization call. By definition in the CCCC standard, the ECM reference location on two-level machines is the first word of ECM (e.g. LCM on the CDC 7600). It should be emphasized that the ECM reference point does not necessarily specify the starting location of ECM.

Except for the implementations on the CDC and CRAY computers (see sections 4.4.3.2 and 4.4.3.3), DRED/DRIT call REED/RITE to perform the random access I/O operations. Consequently, the implementation of DRED/DRIT on IBM 370 systems is simply the REED/RITE implementation discussed earlier in this section.

4.3.4.4 CRED/CRIT

CRED and CRIT are the CCCC routines specified for data string transfer between ECM and FCM. The calling sequence for CRED is:

```
CALL CRED ( FCM(I), LECM, NWDS, IER )
```

This call transfers NWDS single precision words starting from ECM location LECM to the FCM locations starting at the address of FCM(I). IER is an error sentinel. A similar call to CRIT performs the inverse operation.

The implementation of CRED/CRIT on the CDC 7600 employs the COMPASS assembly language routines WRITEC and READEC to perform the actual data transfers between ECM and FCM. The three arguments in the calling sequence for WRITEC are identical in type to the first three arguments in the CRIT calling sequence (e.g. CALL WRITEC (FCM, LECM-1, NWDS)).

The second parameter LECM in CRIT denotes an ECM location relative to the ECM reference array, while the second parameter supplied in the WRITEC call denotes the corresponding ECM address (e.g. LECM-1). On one-level implementations CRED and CRIT simply transfer data between FCM and pseudo ECM locations both of which reside in the same memory level. The transfers are performed via standard Fortran assignment statements.

As noted in the DOPC and DRED/DRIT section, CRED/CRIT are interlocked with DOPC to ensure that the ECM container reference address pointers have been initialized by DOPC.

4.3.4.5 ECMV

ECMV is the CCCC routine specified for transfering data strings between locations in ECM on two-level machines (e.g. CDC 7600). Transfers are performed using CRED and CRIT which route data through a 64-word FCM buffer array local to ECMV. This approach circumvents the compiler restriction limiting array sizes to 131071 words on the CDC 7600. The calling sequence for ECMV is:

```
CALL ECMV ( LECM1, LECM2, NWDS )
```

This call transfers NWDS single precision words starting from ECM location LECM2 to the ECM location starting at LECM1.

4.3.5 BPOINTER, a Dynamic Storage Allocation Program

The problem size limitations imposed by fixed-dimension arrays in a large scale code such as DIF3D is intolerable. Running small problems with unnecessarily large dimensions can be needlessly expensive. Code changes may be awkward and, from a quality assurance standpoint, risky. DIF3D, therefore, uses a dynamic storage allocation system to manage the core storage of data during execution. Core storage is reserved for a particular dimensioned array only during the time the corresponding data are required to be in-core; at other times the space is made available for the storage of other data.

The ARC System dynamic storage allocation routines are contained in the BPOINTER package[36,41]. BPOINTER is a collection of subprograms which was developed to alleviate bookkeeping chores associated with the use of dynamic storage allocation techniques. These chores are separated into two functional categories:

1. The highly machine-dependent functions of obtaining/releasing large blocks of workspace called "containers" from/to the operating system.

2. The largely machine-independent bookkeeping functions associated with managing array allocations within a given container.

Category 1 tasks are performed by the IGTLCM package, a self-contained set of subroutines that may be used independently of BPOINTER. Consequently, in situations requiring only the IGTLCM functions (e.g. the XCM container allocation in the CDC 7600 implementation of DOPC and DRED), inclusion of the BPOINTER routines is unnecessary.

4.3.5.1 Programming Considerations

Programs which use the BPOINTER capability tend to be structured in subroutine form. A control routine is used to define one or two blocks of storage (the containers) and to make the appropriate calls to BPOINTER to control the allocation of space within these containers. Calls to calculational subroutines transmit pointers corresponding to array locations through

the calling sequences. All BPOINTER capabilities are accessed through an appropriate call to an entry point, subroutine or function subprogram. The following capabilities are available in the BPOINTER system:

1. Storage of data in and retrieval of data from the container array via user defined variable arrays.

2. Purge of variable arrays stored in the container array.

3. "Cleanup" of the container array when more storage is required (to avoid fragmentation).

4. Redefinition of array sizes without loss of data already stored in the array.

5. Dump of selected integer, floating point or Hollerith arrays in an appropriate format.

6. Trace edits of BPOINTER activities.

7. Status reports of the BPOINTER tables.

Detailed program documentation including flow charts, common block information and subprogram descriptions is available in Reference 36. A shorter, functional writeup is included in Appendix A of Reference 41 (member POINTR) and gives calling sequences for the BPOINTER routines. This section is intended to provide a brief description of how the program package operates.

The short example shown in Figure 4.8 illustrates the structure of a program using the BPOINTER package. This example demonstrates the manner in which a container is allocated, pointers defined and used, and the container released.

The letters M and B are used as mnemonics within BPOINTER to designate routines which operate on the FCM and ECM containers, respectively. Thus PUTM allocates an array in the FCM container while PUTB allocates an array which must be referenced on a CDC 7600 as either a LEVEL 2 or a LEVEL 3 array. According to CCCC conventions[6], arrays allocated in ECM are referenced through the standard subroutines CRED/CRIT and DRED/DRIT in exportable source code intended for two-level computers.

On IBM equipment without HIARCHY support (e.g. the 370/195) the two containers are both in fast core. The distinctions noted above between the two dynamic containers are important on the CDC 7600 where the containers are addressed quite differently and on IBM equipment with HIARCHY support where access to the LCM container (HIARCHY 1, subpool 1) is significantly slower than access to the MAIN core container (HIARCHY 0, subpool 2).

In the example all dynamically allocated FCM arrays are addressed relative to the labeled COMMON block /ARRAY/ which contains a single array element, BLK(1). In the short-word version of the code the element must be declared REAL*8. In the two-level (CDC 7600) version of BPOINTER the ECM container is addressed relative to the first word of LCM. The pseudo ECM container on IBM equipment is a second container which may be given a HIARCHY 1 location but is

```
CSW
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*4 BLK4
CSW
      COMMON/ARRAY/BLK(1)
      COMMON/IOPUT/NIN,NOUT,NOUT2
      DIMENSION BLK4(1)
      EQUIVALENCE (BLK(1),BLK4(1))
      DATA FLUX/4HFLUX/, POWER/5HPOWER/, MAXSIZ/10000/, NG/27/,
     1 I4/4/, I8/8/, I0/0/
      NOUT=6
C  ALLOCATE CONTAINER WITH MAXSIZ WORDS OF FCM AND NO ECM.
      CALL BULK(I0)
      CALL POINTR(BLK,MAXSIZ,I0)
C  ALLOCATE SPACE FOR ARRAYS POWER AND FLUX.  DETERMINE THE
C  POINTER FOR SUB-ARRAY CURRENT WHICH FOLLOWS THE FIRST NG
C  SINGLE-PRECISION WORDS FOR THE ARRAY FLUX.  THEN CHECK FOR
C  A BPOINTER ERROR.
      CALL PUTM(POWER,NG,I8,IPOWR)
      CALL PUTM(FLUX,2*NG,I4,IFLUX)
      ICURNT=IPT2(IFLUX,NG,I0)
      IF( IPTERR(DUMMY).LE.0 ) GO TO 10
      PRINT 500
  500 FORMAT(15HOBPOINTER ERROR)
      STOP
   10 CONTINUE
C  CALL SUBROUTINE INIT TO USE THESE ARRAYS.  THEN FREE THE
C  CONTAINER AND STOP.
      CALL INIT(BLK(IFLUX),BLK(IPOWR),BLK4(ICURNT),NG)
      CALL FREE
      STOP
      END
C
C-----------------------------------------------------------------
C
      SUBROUTINE INIT(PHI,POWER,CURENT,NG)
CSW
      REAL*8 POWER
CSW
      DIMENSION PHI(1), POWER(1), CURENT(1)
      DO 10 I=1,NG
      PHI(I)=1.0
      POWER(I)=3.1E+06
      CURENT(I)=.333
   10 CONTINUE
      RETURN
      END
```

Fig. 4.8. A BPOINTER Example

addressed in precisely the same manner as the first (FCM) container. The one word assigned to the container by the applications program provides a reference address. At execution time the function routines IGTLCM and IGTSCM are used to obtain the addresses of core which are available to the program for the allocation of data arrays.

A few codes at the same time use BPOINTER and directly address ECM on two-level machines. In these programs the "LEVEL 2" BPOINTER reference common block must start at the first word of LCM. BPOINTER calculates address offsets based on that assumption. DIF3D and most codes currently under development do not address ECM directly; they employ CRED and CRIT to transfer blocks of data between the two levels of memory.

Occasionally it is convenient to exercise the two-level implementation on a one-level machine. In such cases it is necessary to precede the BPOINTER initialization call by the DOPC initialization call so that the user reference address of the BPOINTER ECM container is initialized prior to the first call to CRED/CRIT (BPOINTER employs CRED/CRIT in its two-level implementation). A discussion of IGTLCM/IGTSCM and the associated assembler routines that allocate these blocks of memory follows.

4.3.5.2 IGTLCM/IGTSCM/IGTXCM

Function IGTLCM and its associated entry points IGTSCM and IGTXCM manage the allocation of the ECM, FCM and XCM containers, respectively. The FCM container always resides in fast memory (e.g. the FCM storage pool). The ECM container and the auxiliary ECM container named XCM both reside in the same storage pool. On single-level machines they reside in the FCM storage pool along with the FCM container; on two-level machines like the CDC 7600 they reside in LCM. If the C1LV language flag is activated in a CDC 7600 implementation then the ECM and XCM containers will be allocated in the FCM storage pool along with the FCM container.

IGTLCM, IGTSCM and IGTXCM route all memory allocation requests through function subroutine JGT which calls the appropriate assembler, Fortran or system routines. The calling sequence for IGTLCM is:

```
LOCECM = IGTLCM( NWORDS )
```

This call returns the (REAL*4) word address of the requested block of NWORDS which constitutes the ECM container. A similar call to IGTSCM or IGTXCM allocates the appropriate container. The function value of -1 is returned if the container allocation fails. Subroutine FRELCM with associated entry points FRESCM and FREXCM release the corresponding containers. The example in Figure 4.9 illustrates the use of the IGTLCM package. The function LOCFWD provides the (REAL*4) word address of the reference variable used to address the container.

4.3.5.3 IBM Allocation

The assembler routine MYLCM with entry point MYSCM, FREELC and FREESC (called by JGT or FRELCM) uses the standard IBM macro instructions GETMAIN and FREEMAIN to allocate and free consecutive words of core which are available to the program. The designations subpool 1 and 2 are assigned to the ECM and

```
      COMMON /REFFCM/ BLK(1)
C
C     ALLOCATE FCM CONTAINER
C
      LOCFCM = IGTSCM( NWORDS )
      IF ( LOCFCM .EQ. -1 ) GO TO 10
C
C     DETERMINE WORD OFFSET OF CONTAINER FROM REFERENCE ARRAY BLK(1)
C
      LFCREF = LOCFCM - LOCFWD ( BLK(1) )
C
C     INITIALIZE CONTAINER
C
      DO 1 I=1,NWRDS
      BLK(LFCREF+I)=0.0
    1 CONTINUE
      .
      .
      .
C
C     FREE CONTAINER
C
      CALL FRESCM
      .
      .
      .
C
C     ERROR EXIT
C
   10 CONTINUE
      .
      .
```

Fig. 4.9. IGTSCM/FRESCM/LOCFWD Example

FCM containers, respectively. Since allocations are performed in units of 256 (REAL*8) words, it is most efficient to request blocks of memory in such multiples.

Figure 4.10 shows a schematic diagram of a program and SCM container.

4.3.5.4 CDC Allocation

The COMPASS assembler routine JGTSCM with entry point JGTLCM (called by JGT) uses the standard CDC macro instruction MEMORY to determine and to change the job's SCM and LCM field lengths.

The FCM container is placed at the end of the user's SCM field length, as shown in Figure 4.10. The ECM container is placed at the end of the user's LCM field. The last word of each container is four words short of the user's SCM or LCM field length; this is done to avoid I/O problems in systems that attempt to read ahead. The XCM container is allocated to provide space for indices to the random access records of the DOPC files on the CDC 7600 implementation, only. The implementation uses mass storage routines (READMS, WRITMS, OPENMS and CLOSMS) in the CDC library.

BPOINTER releases containers when they are no longer needed and returns field lengths to their original values.

4.3.5.5 CRAY Allocation (CTSS)

Two subroutines (LASTMEM and MEMORY) from the CRAY Time Sharing System (CTSS) Fortran Library at Los Alamos National Laboratory are called by JGT to determine and change a job's field length, respectively. JGT establishes the user program length (i.e. the high limit of user code, JCHLM) by an initial call to LASTMEM. Each time a new container is requested JGT allocates space in one of two ways:

1. If another container has been previously allocated, and there is enough free space between it and the program, the new container is established in the free space. The field length is not changed.

2. If adequate free space is not available MEMORY is called to increase the field length, and the new container is placed such that the address of its last word is the new value of JCHLM.

Figure 4.11 shows a schematic diagram of fast core of a CRAY machine containing a program and two containers.

JGT reduces the field length by an appropriate amount only when the container ending at address JCHLM is released.

4.3.5.6 CRAY Allocation (COS)

Dynamic memory allocation on machines using the standard CRAY Operating System (COS) is implemented in a manner that is functionally equivalent to the CTSS implementation. CTSS subroutines MEMORY (2 arguments) and LASTMEM are simulated on COS installations by the Fortran subroutine MEMGET and its entry point LASTMEM, respectively. A blank COMMON array of length 1 must be located as follows in order for it to provide a reference point (JCHLM) for the dynamic memory allocation:

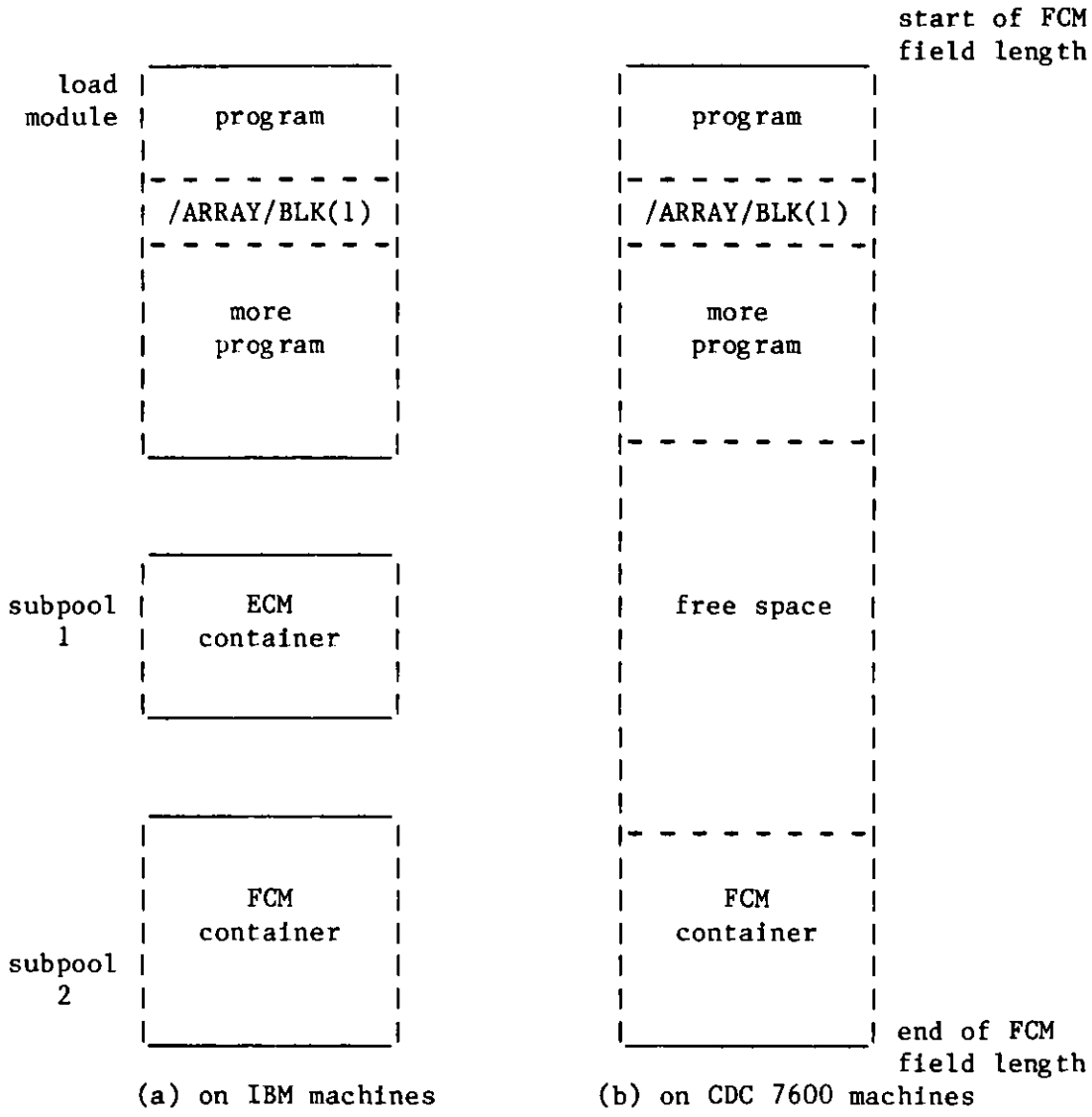

Fig. 4.10. Fast-Core Allocation on IBM and CDC 7600 Machines

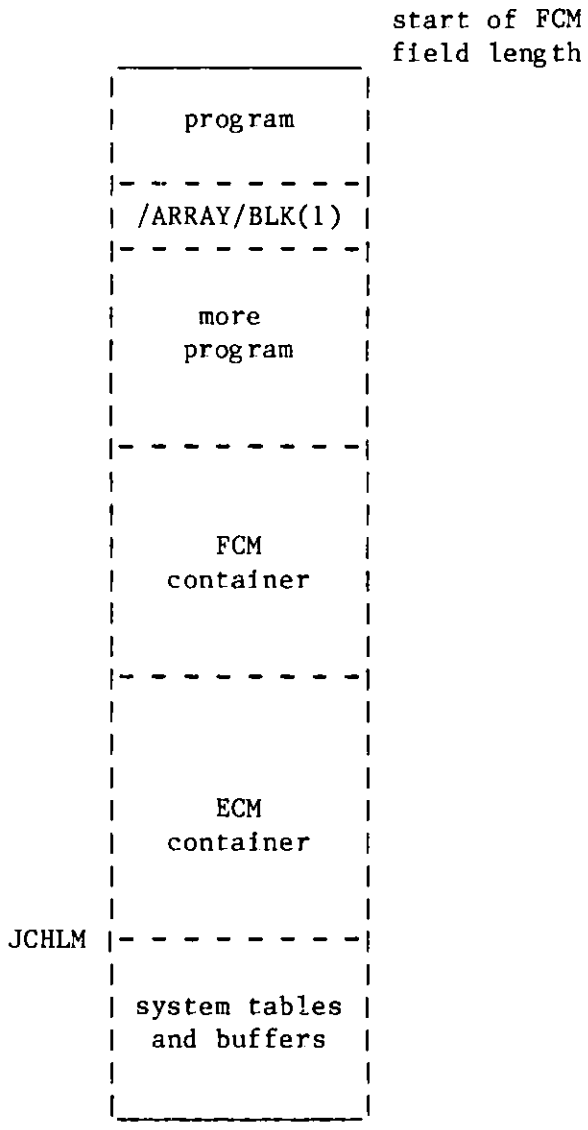

Fig. 4.11. Fast-Core Allocation on a CRAY Machine

1. Non-overlayed COS systems - place it after all object code (the CFT compiler does this by default).

2. Segmented loading on COS system - assign it to a second memory level above all overlays.

3. COS overlay loading types 1 or 2 - assign it (via the SBCA overlay directive) to a specified address larger than any address used in the overlay structure (this number is installation dependent and must be determined upon completion of loading).

Subroutine MEMGET calls the COS system routine MEMORY (5 arguments) which issues calls to the CAL assembler MEMORY macro to increment or decrement JCHLM, the length of the user code area. A corresponding field length change occurs simultaneously.

4.4 Machine Dependence, Hardware and Software Requirements

4.4.1 General Considerations

Machine dependent features in DIF3D that are not universally supported in FORTRAN '66 compilers are isolated in accordance with the coding conventions established by the CCCC[6]. All data transfer, except for BCD input file processing is performed via the CCCC utility routines described in Section 4.3.4. Dynamic storage allocation of FCM and ECM containers is isolated in the IGTLCM routines (Section 4.3.5.2). The BPOINTER package manages the dynamic suballocation of arrays within the ECM and FCM containers. Differences of a global nature such as word length, compiler dialects or machine storage hierarchy are surrounded with pairs of special "keyword" comment cards[41] that are activated or deactivated depending upon the characteristics of the target machine.

4.4.2 Storage Requirements

Formulas for calculating required ECM and FCM container space are given in Tables 3.2 and 3.3. At least 325K-bytes of storage are recommended for program and file buffer storage on the IBM 370 series; 40,000 words of SCM are required on the CDC 7600. ECM requirements are linearly dependent on the number of cells (N) in a mesh plane. The finite-difference option requires at least 9N (8-byte) words in 2-D problems and at least 25N words in 3-D problems. At least 19 mesh lines of data and one group of cross section data must be stored in SCM on the CDC 7600. External data storage must be available for approximately 40 scratch and interface files. Fourteen of these are random access scratch files (grouped into six file groups), the remainder are sequential access files with either formatted or unformatted record types.

4.4.3 Data Access Modes

The calling sequences in the CCCC utility routines REED/RITE and DRED/DRIT provide for asynchronous, sequential and random access I/O. These features have been fully exploited on IBM 370 systems by the SIO package discussed in Section 4.4.3.1 (see also Sections 4.3.4.2 and 4.3.4.3). The READMS, WRITMS, OPENMS and CLOSMS routines provide random access I/O capabilities on CDC 7600 systems (see Section 4.4.3.2). No asynchronous I/O has been implemented on this system. Fortran '77 I/O statements are used to implement random access I/O on the CRAY-1 (see Section 4.4.3.3).

4.4.3.1 SIO, a random access, asynchronous I/O package for IBM systems

In order to make efficient use of large computers such as the IBM System 370 Model 195 or 3033 at Argonne National Laboratory, a program must attempt to optimize both its central processor and peripheral processor operations. Most large scientific programs are written in Fortran, a high level language which provides little flexibility in specifying efficient I/O methods. Several Fortran codes have, however, been designed which would profit by the availability of a program package with the following characteristics:

1. permits asynchronous operation;

2. performs random access operations efficiently;

3. handles large records efficiently;

4. performs I/O operations without the need for buffers.

The SIO program package was written to provide a Fortran-callable access method with these characteristics.

The two IBM-supplied Fortran I/O programs which come closest to satisfying these requirements are the Fortran IV (H Extended) asynchronous I/O and the Fortran IV Direct Access I/O.

The Asynchronous I/O uses V-type records which include control information in each record. Hence buffers are essential. However, with records longer than two tracks on standard direct access devices, the buffers become essentially useless in increasing I/O efficiency, since almost the entire I/O operation must be completed before the user can access the data. Furthermore, these buffers consume large amounts of core, and additional central processor effort is required to move the data between program locations and the buffer. In addition to buffering the data, the Asynchronous I/O operations are sequential and there are no efficient methods for accessing records in a random manner.

Fortran Direct Access I/O does permit random access of the data file, but it is essentially limited to track-length records. This could be overcome through keeping track of the location of each record in an index table and doing software spanning. Since Direct Access I/O uses V-type records, buffering is required. There is also a substantial overhead incurred in the initial formatting of the direct access data set when the file is first opened. Furthermore, asynchronous operation is impossible.

The first step toward attaining a capability with the attributes noted above was to study the IBM I/O routines accessible through standard system Macro calls. Of these, the Basic Sequential Access Method (BSAM) was chosen because it could be used to randomly access records through the Point Macro; it supported U-format records which contain no control information within them; and it features chained scheduling which allows several tracks to be accessed without relinquishing the input/output channel and so decreasing I/O time. As with the Direct Access method, it was necessary to use an index table which contains the relative location of each record and its length. A copy of this table resides in core and also occupies the first track of the

data set. The problem of formatting the data set was overcome by always appending a new record to the end of the data set regardless of which logical record it might be. When records are updated, they are written over the old record if possible, or else appended to the end of the data set like a new record. Asynchronous operation is achieved through subtasking the actual code to do the I/O.

The SIO program package consists of two central modules (SIO and SIOSUB) along with a few auxiliary routines used for edit and error processing (SIOTRC,SIOERR,SIOWU6). In addition the capability may be invoked using the standard I/O routines REED/RITE which branch to the SIO access method for datasets defined with the job control record format U, i.e. RECFM=U. The two main modules consist of a subroutine (SIO) which is included in the main program (task) through appropriate linkage editor control statements and a self-contained load module (SIOSUB) which operates as a subtask after being ATTACHed by the subroutine SIO. There are two assembly parameters in the modules SIO and SIOSUB which are of interest to the user. They are NBLKS and MAXFILES. NBLKS sets the length of the index table discussed above (called the File Control Block or FCB) and determines the maximum number of records which may be placed in the file. For NBLKS=1, 431 entries are allowed; for NBLKS=2, 943 entries are allowed; for NBLKS=3, 1455 entries are allowed; for NBLKS=4, 1967 entries are allowed, but this option is available only if the SIO files are on direct access devices with a track length greater than eight kilbyotes. The parameter MAXFILES specifies the maximum number of files which may be open at a single time. The two parameters are routinely set at NBLKS=2 and MAXFILES=50. The variables must be identically defined both in the main task (SIO) and the subtask (SIOSUB) and files created with a specific value of NBLKS may not be accessed by versions of SIO with a different value of NBLKS.

4.4.3.2 Implementation Considerations on the CDC 7600

Random access I/O on the CDC 7600 is implemented using the routines OPENMS, CLOSMS, READMS and WRITMS found in the Fortran utility library. Auxiliary storage equal in length to the number of records in the file must be supplied during the OPENMS call for each file. An auxiliary ECM container named XCM is allocated directly from DOPC by calling entry point IGTXCM in the IGTLCM dynamic storage allocation subroutine package. Consequently, DOPC and DRED/DRIT depend only on IGTXCM for dynamic storage allocation.

The subscript index limitation of 131071 words imposed on CDC 7600 LCM arrays is effectively raised to 393213 by employing two routines DRED1 and DRED2 each of which addresses a successively higher block of 131070 words of ECM. The circumvention is accomplished by passing the initial address of the next adjacent block of 131070 words of ECM to the appropriate routine, DRED1 or DRED2.

4.4.4 Vectorization on the CRAY-1

Although DIF3D was not designed for a pipelined computer such as the CRAY-1, an advanced computer performance evaluation project[42] at Argonne led to the implementation of a vectorized variant of the SLOR algorithm applicable to nonperiodic, orthogonal geometry models. The regular mesh structure and the fact that at least 75% of the DIF3D scalar execution time is spent in a

small kernel of subroutines that perform the SLOR algorithm provided ample opportunity for vectorizing (with vector lengths J/2) the dominant computations in DIF3D without changing the DIF3D data structure.

The vector pipeline of the CRAY-1 is exploited by simultaneously solving the tridiagonal matrix equations generated for the (J+1)/2 odd lines on a mesh plane, and then simultaneously solving the corresponding tridiagonal matrix equations generated for the J/2 even lines on a plane. This odd/even (red/black) SLOR algorithm[43,44] was implemented within the existing DIF3D data structure by modifying subroutine OSWEEP and by increasing one auxiliary mesh line array (SOLN) to the size of a mesh plane array. The CRAY-1 version of OSWEEP calls RBOSRC and RBOSOR, the vectorized counterparts of the ROWSRC and SORINV subroutines, twice for each mesh plane k before processing plane k + 1; the first pass processes the odd numbered lines on plane k and the second pass processes the even numbered lines.

A comparison of the relative megaflop rates (millions of floating point operations per second) achieved by the scalar (conventionally ordered) and the vector (odd/even ordered) algorithms, when applied to the two-dimensional IAEA benchmark problem with a (170 × 170) rectangular mesh, is tabulated in Table 4.5.

The results[45] in Table 4.5 should be viewed in light of three considerations. First, one expects a factor of 2.3 increase in megaflop rates on the CRAY-1 due to machine clock cycle differences (12.5 nanosecs on the CRAY-1 vs. 28.5 nanosecs on the IBM 370/195). Second, the ROWSRC subroutine in the so-called scalar algorithm will vectorize on the CRAY-1. Third, the megaflop rate of the current, vectorized algorithm is dependent on the problem in two respects. The vector length depends on the number of lines (J) on a plane; the vector stride (the number of memory words between successive vector elements) of length 2I will cause memory bank conflicts whenever

Table 4.5. Execution Rates for the 2D IAEA Benchmark[a]

Method/Machine	Cray-1	IBM 370/195
Vector Fortran (RBOSRC, RBOSOR)	4.4	0.83
Scalar Fortran (ROWSRC, SORINV)	1.6	-
Scalar Fortran with Assembler SORINV	2.7	1

[a]Rates are expressed in units of 3.9 megaflops. The 2 group model is defined with a 1 cm (170 × 170) mesh.

the line length I is a multiple of 8 on the typical 16 memory bank machine. Work in progress towards implementation of a vector length of J·K/2 should yield favorable performance increases for a wider class of problems without significantly altering the DIF3D data structure.

5. THE NATIONAL ENERGY SOFTWARE CENTER VERSIONS OF DIF3D

DIF3D is available on magnetic tape through the National Energy Software Center; versions exist for the IBM 370 series, the CDC 7600 and the CRAY-1 computers. This section describes the contents of the tapes and outlines the steps necessary to implement the code in a standalone form on the above mentioned computers. Knowledge regarding solution techniques or the code itself is not assumed. The NESC package includes several benchmark problems; this section also contains descriptions and solutions of these test problems.

5.1 The DIF3D Package

The NESC package consists of this report and a magnetic tape the characteristics of which are listed in Table 5.1. Tables 5.2 a, b, c respectively describe the contents and approximate length of each BCD file on the tape for each of the three target computers noted above.

TABLE 5.1. DIF3D Tape Characteristics and its BCD File Contents

Characteristics	
Type	9 track
Density	1600 bpi
Label	unlabeled
Block Size	3200 (1596)[a]
Record Length	80 (133)[a]
Format	EBCDIC

[a]Parenthesized quantities apply to sample problem output files only.

5.1.1 File 1 - DIF3D FORTRAN Source Images

The source code in files 1 and, if applicable, files 2 and 3 combine to form the DIF3D code. The first file includes the major code blocks summarized in Table 5.3. FORTRAN source for all machine versions is derived from a single master source file. Statements that are unique to a particular implementation are surrounded by pairs of "keyword" comment cards. Code within the keyword brackets is selectively "activated" (uncommented) or "deactivated" (commented out) by a simple preprocessing program[41] at the time a tape is generated. The keywords bracket coding applicable to general machine architectural features such as long and short word lengths (e.g. CLW or CSW) and one- or two-level memory hierarchies (e.g. C1LV or C2LV). Particular manufacturer, compiler or installation dependencies are also bracketted (e.g. CIBM, CDC*, CRAY, CANL, CLBL and CD76). Keywords (CSA, CSEG and COVL) exist for generating modular or standalone code appropriate for segmented or overlay loading.

This package is sufficiently large that although the source code on the tape will be numbered in a global fashion, future code modifications will be specified on a subroutine basis, only.

TABLE 5.2a. Contents of NESC Export Tape for IBM 370 Systems

File Number	Contents	Estimated Number of Card Images
1	DIF3D FORTRAN Source Code	79196
2	Machine Dependent Source Code	1498
3	SIOSUB Subtask (IBM) Assembler	1228
4	Loader Directives	194
5	ARCSP021 JCL Procedure	282
6	Sample Problem Input (Cases 1, 2, 3 and 4)	226
7	Sample Problem Input (Cases 5 and 6)	161
8	Sample Problem Output (Cases 1, 2, 3 and 4)	3936
9	Sample Problem Output (Cases 5 and 6)	2392
10	CCCC and Code Dependent File Descriptions	5431

TABLE 5.2b. Contents of NESC Export Tape for CDC 7600 Systems

File Number	Contents	Estimated Number of Card Images
1	DIF3D FORTRAN Source Code	79196
2	Loader Directives	121
3	Sample Problem Input (Cases 1, 2, 3 and 4)	226
4	Sample Problem Input (Cases 5 and 6)	161
5	Sample Problem Output (Cases 1, 2, 3 and 4)	3936
6	Sample Problem Output (Cases 5 and 6)	2392
7	CCCC and Code Dependent File Descriptions	5431

TABLE 5.2c. Contents of NESC Export Tape for CRAY-1 Systems

File Number	Contents	Estimated Number of Card Images
1	DIF3D FORTRAN Source Code	79196
2	Machine Dependent Source Code (optional)	177
3	Loader Directives	121
4	Sample Problem Input (Cases 1, 2, 3 and 4)	226
5	Sample Problem Input (Cases 5 and 6)	161
6	Sample Problem Output (Cases 1, 2, 3 and 4)	3936
7	Sample Problem Output (Cases 5 and 6)	2392
8	CCCC and Code Dependent File Descriptions	5431

TABLE 5.3. DIF3D Code Blocks

Principal Code Blocks	Approximate Number of Card-Images
D3DRIV (+ utilities)	9537
SCAN	306
STUFF	730
GNIP4C	23043
HMG4C	4745
MODCXS	938
BCDINP	1176
S4C10A	2625
DIF3D	36056
UDOIT1,2,3,4	40

5.1.2 Machine Dependent Source Code

Most compilers (except for the FTN compilers on the CDC 7600) do not permit the intermixing of FORTRAN and assembler source code. File 2, therefore, segregates assembler code from the FORTRAN coding on File 1 for computers other than the CDC 7600. Some of the assembler code located on File 2 is provided solely for the purpose of optimizing CPU performance, and is optional in this respect.

On the tape destined for IBM installations, file 2 contains IBM assembler code for dynamic storage allocation and for asynchronous, random access I/O processing. File 3 on this tape contains the IBM assembler source code for the SIOSUB subtask which is required for the DIF3D random access I/O implementation on IBM 370 systems. See the explanation in Section 5.4.3.

On the tape destined for the CDC 7600, assembler subroutines for dynamic storage allocation, for transfers between ECM and SCM and for optimizing SORINV (the subroutine which performs the back substitution and overrelaxation tasks in the SLOR solution of the tridiagonal matrix equations) are appropriately located with their FORTRAN counterparts and associated routines on file 1.

File 2 on the CRAY-1 tape contains an assembler coded optimized version of the (non-vectorizable) SORINV routine mentioned in the previous paragraph. Subroutines RBOSOR and RBOSRC for the vectorizable (odd/even ordering) SLOR algorithm are present on file 1 (see Section 4.4.4).

5.1.3 Loader Instructions

Instructions for creating the DIF3D overlay or segment structure are included for the convenience of the user. Linkage editor instructions are provided on the NESC tape for IBM 370 systems (see also Appendix E). Instructions for the SEGLINK segmented loader at Lawrence Berkeley Laboratory are included on the CDC 7600 tape (see also Appendix F.1). Type 01 overlay directives are included with the CRAY-1 tape (see also Appendix F.2). As noted in Section 5.1.1 all tapes have overlay calls and directives present in the FORTRAN source; these are appropriately activated (uncommented) on the CDC 7600 and CRAY-1 tapes (see Section 5.2.1).

5.1.4 Sample Problem Input and Output

Six problem cases are supplied; four of these cases arise from two- and three-dimensional models of the well-known SNR Benchmark Problem[46,47] in four energy groups. Solutions for both the finite-difference triangular geometry option and the nodal hexagonal geometry options are generated for these two models. Two- and three-dimensional models of the well-known IAEA benchmark problem[48] with two energy groups provide the remaining two test problems. Finite-difference solutions of these orthogonal geometry (XY and XYZ) problems are generated. Section 5.3 describes the benchmark problems.

Each sample problem was run on the IBM 370 system at Argonne and the corresponding output, including carriage control symbols, is provided on the NESC tape. The output files will consequently have a record length of 133 characters.

5.1.5 ARCSP021, An Instream JCL Procedure for IBM 370 Systems

ARCSP021, the instream JCL procedure appropriate for running the NESC version of DIF3D on IBM systems is provided for the convenience of the user. It is listed in Appendix A and a discussion of its parameters appears in Section 3.12.3.

5.1.6 CCCC and Code-Dependent Interface File Descriptions

The file descriptions for the various interface files used in DIF3D are provided on the tape to allow the user to inexpensively generate additional copies. These descriptions also appear in the Appendices B, C and D of this report.

5.2 Implementation of the NESC DIF3D as a Stand-Alone Program

5.2.1 Code Structure and Loading Instructions

Table 5.3 lists the major code blocks within the DIF3D code system; functional descriptions of these code blocks appear in Section 4.1. A minimal overlay structure, other than no overlays at all, uses these major code blocks as primary overlays and D3DRIV as the root overlay. A detailed overlay structure is given for the major code blocks GNIP4C, HMG4C and DIF3D in Figures 4.2, 4.3 and 4.4, respectively. On systems restricted to three overlay levels, a root segment with primary and secondary overlays only (e.g. CDC 7600 overlay loader or the type 01 overlay directives on the CRAY-1), subroutine DIF3D is assigned to the root segment as a logical extension of the main driver D3DRIV. This puts the major overlays of the neutronics solution at the same (primary overlay) level as the remaining code blocks GNIP4C, HMG4C, etc.

Source code for the major code blocks is on File 1 of the NESC tape; code generated from assembling the machine-dependent source (if present) on File 2 should be included at load time with the root segment. Loading instructions for the target computers are included in the appropriate files noted in Tables 5.2 a, b, c. Also present within the source code are appropriately inactivated (e.g. commented) or activated (uncommented) overlay directives for the CDC 7600 and CRAY-1 computers. Appendices E, F.1 and F.2 display the job control language and the loader directives required to create the DIF3D load modules for each computer.

SIOSUB, a separate subtask module (file 3), is required to implement the random access I/O capability used by DIF3D on IBM systems. The next section describes its relation to the SIO access method and its placement in the STEPLIB data set prior to execution.

5.2.2 SIO

The SIO access method provides a random access, asynchronous I/O capability on IBM operating systems. Within DIF3D the SIO routines are invoked directly from the CCCC generalized I/O subroutines REED and RITE. The source code for SIO is included as part of the DIF3D standalone code and requires special care with regard to its implementation. In particular, SIO is made up of an assembler language module, SIOSUB, and three assembler subroutines, SIO, RECFM and SIOTRC. The latter routines are assembled and included within the root segment of the DIF3D load module in a manner completely analagous to Fortran routines such as REED and RITE. The subroutine RECFM is called by REED/RITE to interrogate the DCB of a dataset to determine whether it has been designated with an undefined record format, i.e. RECFM=U. If so, it is considered an SIO dataset and the subroutine SIO is called to perform the I/O rather than the Fortran system routine IBCOM#. The subroutine SIO sets up argument lists and then passes control to the load module SIOSUB to perform the actual I/O operations. Thus, in addition to the DIF3D load module, a second load module, SIOSUB, must be available to the system at the time of execution of DIF3D, i.e. SIOSUB must be a member of a partitioned data set referenced in the STEPLIB data definition JCL of the job step. To create the load module SIOSUB, it is necessary to assemble the source code and link edit the resulting object code using standard procedures. It is however essential that the load module SIOSUB be assigned the "Re-enterable" attribute by the linkage editor. This may be done by assigning the parameter RENT in the PARM field of the linkage editor execution step as follows:

```
//LKED        EXEC PGM=IEWL,PARM='RENT,...'
```

5.2.3 File Number Assignments

All sequential binary files (input and output interface files and scratch files) used in the DIF3D code system are handled through the CCCC standard subroutines SEEK, REED and RITE. The assignment of file numbers to file names and the initialization of the SEEK tables is done from the DIF3D driver D3DRIV (also known as MAIN on IBM systems). Subroutine SEEK is also used to obtain reference numbers for sequential BCD interface files; the subroutine SEKPHL is then used to obtain corresponding logical unit numbers for subsequent use with FORTRAN READ and WRITE statements. SEKPHL is also called to rewind (close) all BCD data sets. Section 4.3.4 describes these functions.

Fourteen random access scratch files are exclusively referenced by the CCCC standard subroutines DOPC, DRED and DRIT; only the DIF3D neutronics solution code block references these files. File names RNDM01-RNDM14 correspond to DOPC reference numbers 1-14, respectively. The Argonne implementation of the DOPC, DRED and DRIT package uses subroutine SEEK to assign logical unit reference numbers to the 14 DOPC reference numbers. Except for noted exceptions, all DOPC calls are issued from subroutines SSDISK or NHDISK in the DIF3D initialization segment SSINIT. The exceptions are the DOPC initialization and termination calls in subroutine DIF3D, the driver for the DIF3D neutronics

module proper, and a DOPC call required in subroutine XSREV, the adjoint cross section reversal subroutine. In the latter case, DOPC file group 6 is deleted and redefined with a potentially different record size in its lone member file.

Table 5.4 lists all of the files used by the code blocks in the NESC version of DIF3D and classifies them into one of five different categories that have already been defined in Section 4.2 for the Argonne production version of DIF3D. As shown in the table, printer output is written to file 6 and optionally to file 10. BCD input data is read from file 5; BCD or binary interface files which exist at the start of a job will be read from their respective files. The DOPC data sets in Table 5.4 have previously been defined in Table 4.3.

TABLE 5.4. Data Set Classification for the NESC DIF3D

File Reference Number	File Name	File Type[a]	File Description
5		BCD	input data for SCAN module
6		BCD	output data all modules
9		BCD	input data spool from SCAN
10		BCD	auxiliary output all modules
11	A.DIF3D	BCD	DIF3D control
12	A.NIP3	BCD	GNIP4C control
13	A.HMG4C	BCD	HMG4C control
15	A.ISO	BCD	BCD ISOTXS
18	DIF3D	CDB	DIF3D control
19	COMPXS	CDB	macroscopic cross sections
20	LABELS	CDB	labels, half-heights
22	D3EDIT	CDB	tabular edits spool
23	NHFLUX	CDB	nodal restart (real)
24	NAFLUX	CDB	nodal restart (adjoint)
25	PKEDIT	CDB	peak power/flux interface
26	GEODST	CCCC	geometry description
27	ISOTXS	CCCC	microscopic cross sections
28	NDXSRF	CCCC	nuclide/zone reference
29	ZNATDN	CCCC	zone nuclide atom densities
30	RTFLUX	CCCC	real flux
31	ATFLUX	CCCC	adjoint flux
32	FIXSRC	CCCC	fixed source
33	RZFLUX	CCCC	zone flux averages
34	PWDINT	CCCC	power density
39	SEARCH	CCCC	SRCH4C control
41-56[b]	RNDMnn	DOPC	random access scratch files
66-71	SCR001-6	SCR	scratch files
76-78	UDOIT	CDB	UDOIT versions 1-3
80	AUDOIT	BCD	UDOIT module input

[a]See Section 4.2. CDB denotes a code-dependent binary file.

[b]Table 4.3 describes the 14 DOPC files. Reference numbers 44 and 50 are undefined.

File assignments may be easily reassigned by changing source code in D3DRIV; no other routines need be modified. All files are written sequentially (one minor exception is noted in Section 4.4.3; it applies to adjoint calculations with upscatter). If necessary, all files may be read sequentially. Greater efficiency is achieved when random access I/O methods are employed. Reading the flux file in the inscatter source calculation and the flux and finite-difference coefficient files during the concurrent inner iteration strategy are the principal I/O operations affected by this access method.

5.2.4 Running the NESC version of DIF3D

DIF3D is designed to run in environments in which codes that follow the CCCC standards may have never before been implemented. If desired, all input data may be entered in BCD form. BCD input processors within the DIF3D code system will subsequently convert this data to the necessary CCCC and code-dependent binary interface files. Existing BCD or binary interface files will also be accepted by DIF3D. Table 4.2 summarizes the input and output interface files for each code block within the DIF3D code system. The contents and formats of the BCD and binary interface files are given in the interface file descriptions in Appendices B-D. The sample problem input data on the NESC tape is entirely in BCD format.

The BCD data format principally consists of sets of card images having a two-digit card type identifier in columns 1 and 2. Frequently, several cards of the same type are required; the ordering of cards within a given type is usually fixed. Data associated with a particular file is preceded by the card image DATASET=filename and terminated by another DATASET=filename card for the next file, by a BLOCK=STP021 card or by an end-of-file indicator. Alternative keywords to DATASET (e.g. UNFORM, NOSORT and MODIFY) are described in Section 3.2; these provide free field input, special dataset treatment (e.g. A.ISO), and permit modification of specified card types (replacement or deletion), respectively. Preceding a collection of DATASETs must be a BLOCK= STP021 card image. Each such BLOCK invokes another execution of DIF3D. Old DATASETS (files) which already exist at the start of a job are specified in the BLOCK=OLD block. The list of old DATASETs consists of card images of the form DATASET=filename.

Most systems require users to specify memory size and CPU time estimates in a JOB control statement (see JOB Control examples in Section 3.12, Figs. 3.5, 3.8 and 3.9). DIF3D jobs require a fixed amount of storage to contain the longest program overlay and I/O buffers, and a problem-dependent minimum amount of computer memory for the FCM and ECM data storage containers (see Section 3.9). The FCM and ECM container sizes specified in the sample problem input are appropriate for the CDC 7600, but they may also be used (less efficiently) on the other target computers. The length of the longest overlay is installation dependent and can be obtained by examining the output from a successful loader job. The amount of space required for I/O buffers is also installation and implementation dependent; at a given moment the maximum number of files that are opened is problem dependent, but should not exceed 14 (the number of DOPC files). This number does not include the three BCD input and output file unit numbers 5, 6 and 10. A practical estimate may be closer to 6 or 7 simultaneously open files.

For IBM and CRAY-1 systems region sizes specified on the JOB card provide an upper bound on the allowable memory to be used for both program instructions and dynamically allocated storage containers. On the CDC 7600, the FCM and ECM field length requests should only include space required for the longest overlay; additional space will be dynamically allocated via calls to IGTLCM or IGTSCM from the BPOINTER package. The sample problem discussions which follow include container size and CPU time estimates for each problem.

5.3 Sample Problems

Six problem cases are derived from two benchmark source situations. Summarized in Table 5.5 are estimates of typical FCM and ECM container sizes that are appropriate for running the sample problems on the designated computers. For implementations on the IBM 3033 or CRAY-1 computers these estimates may optionally replace the container sizes (on the A.DIF3D type 02 card) supplied with the sample problems on the NESC tape. As noted above the supplied sizes are appropriate for the CDC 7600. The relatively large container sizes suggested for the CRAY-1 (operating under the CRAY Time Sharing System at Los Alamos National Laboratory) reduce expensive I/O costs in favor of less expensive memory residence charges. Because sample problems 1-4 are combined in a single job (as are sample problems 5-6), JOB region size or field length calculations are governed by the largest container sizes in each problem set (i.e. problems 4 or 6).

5.3.1 The SNR Benchmark Problem

The SNR benchmark problem[46,47] is a 4-group model of a 300 MWe homogeneous-core LMFBR originally specified in both Cartesian and triangular geometry. The modified problem[5,47] solved here is obtained by altering the outer boundary of the triangular-geometry model (while preserving the volume of the core) to allow imposition of boundary conditions along surfaces of hexagons. The model consists of a two-zone core surrounded by radial and axial blankets without a reflector. The height of the active core is 95 cm, and each axial blanket is 40 cm thick. A total of 11 rings of hexagons (including the central hexagon) are included in the model, with a lattice pitch of 11.2003 cm. $J_{in}=0$ boundary conditions are imposed on the outer surfaces of the blankets. The full-core model includes a total of 18 control rods, with 6 of these rods parked at the core-upper axial blanket interface, and the remaining 12 inserted to the core midplane. As in Ref. 5, all calculations are performed using sixth-core symmetry.

5.3.1.1 The Two-Dimensional Model

Figure 5.1 displays the BCD input data contained on the NESC tape for the two-dimensional SNR benchmark problem. Two cases corresponding to the finite-difference and the nodal solution options are specified. Data following the second BLOCK=STP021 in Fig. 5.1 invokes the nodal solution option. The REMOVE=filename cards located after the second BLOCK=STP021 card turn off the existence sentinels for the corresponding file names in the SEEK table before processing begins for the second case. Selected printed and plotted output from these two cases is displayed in Appendices G.1 and G.2. Included are a geometry map, a mesh cell to region map, macroscopic cross section edits and tabulations of region and area integrals for power density, total flux and neutron balances.

TABLE 5.5. Resource Estimates for Sample Problems 1-6

Problem and Computer	Container Size FCM	ECM	CPU Time (Seconds)[b]
Sample 1 - 2D SNR Finite Difference Option			
IBM 3033	450	4300	2.8
CDC 7600	3600	6000	1.7
CRAY-1	550	11250	1.9
Sample 2 - 2D SNR Nodal Option			
IBM 3033	550	5700	1.8
CDC 7600	4000	5700	1.0
CRAY-1	600	6100	1.6
Sample 3 - 3D SNR Nodal Option			
IBM 3033	600	27000	21
CDC 7600	20000	27000	11
CRAY-1	650	61000	11
Sample 4 - 3D SNR Finite Difference Option			
IBM 3033	550	15300	147
CDC 7600	12000	164000	81
CRAY-1	650	450000	42
Sample 5 - 2D IAEA Problem Finite Difference Option			
IBM 3033	800	62000	60
CDC 7600	20000	102000	25
CRAY-1	8040	102000	11
Sample 6 - 3D IAEA Problem Finite Difference Option			
IBM 3033	400	94000	74
CDC 7600	8000	166000	36
CRAY-1	800	166000	19

[a]Units are decimal number of longwords (REAL*8 words on IBM systems). JOB region size calculations are given by:

IBM 3033: REGION = 325K + (FCM + ECM)/(128 words/K byte)
CDC 7600: SCM = $100{,}000_8$ + FCM (octal words)
LCM = SCM + ECM + buffers (octal words)
CRAY-1 : REGION = 200000 + FCM + ECM (decimal words) (unoverlayed)

[b]CPU times on the IBM 370/195 are approximately 30 to 50% less than on IBM 3033.

```
//SNR2D3D  JOB REGION=1700K,TIME=8,CLASS=X
//*MAIN    LINES=25,ORG=PRO
// EXEC    ARCSP021
//SYSIN DD *
BLOCK=STP021
UNFORM=A.DIF3D
01    **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FD06
02    1600  8500
03    0 0 0 4500 50
04    1 0 0 11 111 10 100 1 0 0
05    1.0E-10 1.0E-10 1.0E-10
06 1.0 0.001 0.04 0.5
UNFORM=A.NIP3
01    **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FD06
02    0  1 10000  0  500  0  0  0  0  1
03    70
04    7 4 0 4
05    XU  .5000  1 4
05    YU  .5000  1 4
14    M1    I1    1.0
14    M2    I2    1.0
14    M3    I3    1.0
14    M4    I4    1.0
14    M5    I5    1.0
14    M6    I6    1.0
15    M1    IC
15    M2    OC
15    M3    RB
15    M5    CR
15    M6    CF
29    11.2003  11  1
30    IC  1
30    IC  2
30    IC  3
30    IC  4
30    IC  5
30    IC  6
30    OC  6  1
30    OC  7
30    OC  8
30    RB  9
30    RB 10
30    RB  8  1
30    OC  9  4  5
30    OC  9 45 46
30    RB 11  5  6
30    RB 11 56 57
30    CR  7  3
30    CR  7 35
30    CF  4  1
NOSORT=A.ISO
 OV ISOTXS  HH2  *GFK 3D BNCH *     1
 1D      4     6     0     3     0     1     1     1
 2D *NA COOLED FBR BENCHMARK FOUR GROUP CROSS SECTIONS                *
*      * I1      I2      I3      I4      I5      I6
0.768      0.232      0.0          0.0
1.72336E+09 4.02463E+08 7.97003E+07 3.15946E+07 1.05    E+07 8.00    E+05
10000.       1000.       0.0
    0     3     6     9    12    15
4D  I1      GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .11587      .21220      .46137      .34571      .11587
.21220      .46137      .34571      .69059  E-031.830758E-03 .92948 E-02
.17305 E-01 .39123 E-02 .18286 E-02 .36334 E-02 .92415 E-02 3.036066
2.912173    2.881874    2.879511
7D 0.0          0.0          .023597     0.0          .16153  E-02
.40791 E-05 0.0          .46838 E-02 .42309 E-07 .44493 E-07
4D  I2      GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .11588      .21213      .46770      .35349      .11588
.21213      .46770      .35349      .66221 E-031.83956 E-03 1.00354E-02
.20476 E-01 .48531 E-02 .26377 E-02 .51332 E-02 .13238 E-01 3.079063
2.914926    2.884945    2.882535
7D 0.0          0.0          .023262     0.0          .15718  E-02
.46451 E-05 0.0          .43414 E-02 .40724 E-07 .49968 E-07
4D  I3      GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .14584      .28443      .52703      .40732      .14584
.28443      .52703      .40732      1.11527E-033.063463E-031.002116E-02
.129995E-01 .27688 E-02 .44347 E-04 .12274 E-03 .34952 E-03 2.796410
2.440977    2.423171    2.422951
7D 0.0          0.0          .032071     0.0          .27776  E-02
.38880 E-05 0.0          .58971 E-02 .90018 E-07 .45039 E-07
4D  I4      GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .12270      .23133      .46274      .33749      .12270
.23133      .46274      .33749      8.2278 E-042.170873E-03 7.64083E-03
.97185 E-02 .19453 E-02 .31065 E-04 .87566 E-04 .23769 E-03 2.790264
2.441880    2.423086    2.422988
7D 0.0          0.0          .026322     0.0          .22889  E-02
.28907 E-05 0.0          .53536 E-02 .62133 E-07 .33248 E-07
4D  I5      GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     0     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .13317      .25355      .58044      .54168      .13317
.25355      .58044      .54168      .186696E-02 .126433E-01 .634405E-01
.16868
7D 0.0          0.0          .022946     0.0          .37687  E-02
.10320 E-05 0.0          .86815 E-02 .70361 E-11 .10489 E-07
```

Fig. 5.1. Input Data for the Four SNR Benchmark Problem Models

```
4D  I6      GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     0     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .072206      .11487       .32642       .19272       .072206
.11487       .32642       .19272       .216305E-03 .16880 E-03 .11468 E-02
.78660 E-03
 7D 0.0          0.0          .012942      0.0          .12871  E-02
.66780 E-06 0.0          .34533 E-02 .43633 E-11 .69903 E-08
BLOCK=STP021,3
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
MODIFY=A.DIF3D
01     **** SAMPLE PROBLEM 2 ****   2D SNR BENCHMARK - RODS IN - NODAL
02      600  5500
11     1 40.0 1 87.5 1 135.0
11     1 175.0
UNFORM=A.NIP3
01     **** SAMPLE PROBLEM 2 ****   2D SNR BENCHMARK - RODS IN - NODAL
03     114
BLOCK=STP021,3
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
REMOVE=NHFLUX
REMOVE=DIF3D
UNFORM=A.DIF3D
01     **** SAMPLE PROBLEM 3 ****   3D SNR BENCHMARK - RODS IN - NODAL
02     2000  60000 0
03     0 0 0 4500 30
04     1 0 0 00 110 10 100 1 0 0
05     1.0E-7  1.0E-5  1.0E-5
06     1.0 0.001 0.04 0.5
11     1 40.0 1 87.5 1 135.0
11     1 175.0
UNFORM=A.NIP3
01     **** SAMPLE PROBLEM 3 ****   3D SNR BENCHMARK - 8 PLANES - NODAL
02     0  1  8000   0 500  0  0  0  0  0
03     124
04     7 4 0 4 4 4
05     XU  .5000  1 4
05     YU  .5000  1 4
05     ZL  .5000  1 4
05     ZU  .5000  1 4
09     Z 2 40.0 2 87.5 2 135.0
09     Z 2 175.0
14     M1     I1     1.0
14     M2     I2     1.0
14     M3     I3     1.0
14     M4     I4     1.0
14     M5     I5     1.0
14     M6     I6     1.0
15     M1     IC
15     M2     OC
15     M3     RB
15     M4     AB
15     M5     CR
15     M6     CF
29     11.2003  11  1
30     AB    1  0  0   0.0 175.0
30     IC    1  0  0  40.0 135.0
30     AB    2  0  0   0.0 175.0
30     IC    2  0  0  40.0 135.0
30     AB    3  0  0   0.0 175.0
30     IC    3  0  0  40.0 135.0
30     AB    4  0  0   0.0 175.0
30     IC    4  0  0  40.0 135.0
30     AB    5  0  0   0.0 175.0
30     IC    5  0  0  40.0 135.0
30     AB    6  0  0   0.0 175.0
30     IC    6  0  0  40.0 135.0
30     AB    7  0  0   0.0 175.0
30     OC    7  0  0  40.0 135.0
30     AB    8  0  0   0.0 175.0
30     OC    8  0  0  40.0 135.0
30     RB    9  0  0   0.0 175.0
30     RB   10  0  0   0.0 175.0
30     AB    6  1  1   0.0 175.0
30     OC    6  1  1  40.0 135.0
30     RB    8  1  1   0.0 175.0
30     AB    9  4  5   0.0 175.0
30     OC    9  4  5  40.0 135.0
30     AB    9 45 46   0.0 175.0
30     OC    9 45 46  40.0 135.0
30     RB   11  5  6   0.0 175.0
30     RB   11 56 57   0.0 175.0
30     CF    4  1  1   0.0 135.0
30     CF    7  3  3   0.0  87.5
30     CF    7 35 35   0.0  87.5
30     CR    4  1  1 135.0 175.0
30     CR    7  3  3  87.5 175.0
30     CR    7 35 35  87.5 175.0
BLOCK=STP021,3
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
REMOVE=NHFLUX
MODIFY=A.DIF3D
01     **** SAMPLE PROBLEM 4 ****   3D SNR BENCHMARK - RODS IN - FD0636
MODIFY=A.NIP3
01     **** SAMPLE PROBLEM 4 ****   3D SNR BENCHMARK - RODS IN - FD0636
03     90
09     Z 8 40.0 10 87.5 10 135.0
09     Z 8 175.0
```

Fig. 5.1. Input Data for the Four SNR Benchmark Problem Models (contd.)

5.3.1.2 The Three-Dimensional Model

The third and fourth BLOCK=STP021 cards in Fig. 5.1 signal the start of the three-dimensional models solved by the nodal and finite-difference options, respectively. The MODIFY=filename cards permit selective modification of card types within appropriate data sets; previously existing data that are still pertinent need not be respecified. Appendices G.3 and G.4 display selected printed output for these two cases.

5.3.2. The IAEA Benchmark Problem

The IAEA benchmark problem[48] is the well-known 2-group LWR model designed as a severe test for the capabilities of coarse mesh methods and flux synthesis approximations. The problem solved here has the $J_{in}=0$ boundary condition applied at external boundaries. Because the DIF3D finite-difference option requires a rectangular boundary domain in the XY plane, the irregular outer boundaries on the XY plane that are required by the benchmark specifications are modelled by assigning the inactive mesh cells to a blackness theory region with an appropriate internal black boundary condition constant (B=.5). The dimensions of the quarter-core planar model are 170 × 170 cm. The three-dimensional quarter-core model has 380 cm in the axial dimension. Two fuel regions, a reflector and five inserted rods (one of which is only partially inserted) appear in the quarter-core model.

5.3.2.1 The Two-Dimensional Model

Input data for the two-dimensional IAEA problem appear in Figure 5.2. Printed and graphical output selections similar to those chosen for the SNR problems are displayed in Appendix G.5.

5.3.2.2 The Three-Dimensional Model

Input data for the three-dimensional IAEA problem also appear in Figure 5.2; it follows the second BLOCK=STP021 card. Selected printer output is displayed in Appendix G.6.

5.4 Suggested Local Modifications

The export package described in this chapter is designed to run in standalone fashion on a variety of machines and operating systems. Because of this we cannot take advantage of local system routines and options. In this section we point to several areas of the code which programmers may wish to modify to make DIF3D more compatible with the local system.

5.4.1 SEEK Initialization

The initialization of the SEEK tables at the front of the driver of the code is done in the manner required by the version of SEEK which accompanies the NESC package. Programmers at those installations that have their own version of SEEK may wish to modify the initialization procedure coded into the DIF3D driver. There are no CCCC standards for SEEK initialization.

```
BLOCK=STP021
UNFORM=A.DIF3D
01     **** SAMPLE 5 ****  IAEA 2D BENCHMARK - 2. CM MESH
02 20000 102000
03 0 0 0 0 50
04 1 0 0 11 110 10 100 1 1
06 0. 0. .01
UNFORM=A.NIP3
01     **** SAMPLE 5 ****  IAEA 2D BENCHMARK - 2. CM MESH
02 0 1 17000 0  2000
03 40
04 3 4 3 4
05 0. .5 0. .5
06 RREFL    0. 170.  85  85   0. 170.
06 RFUEL1   0.  50.  25  20 110. 150.
06 RFUEL1  50.  90.  20  20  90. 130.
06 RFUEL1  90. 110.  10  10  90. 110.
06 RFUEL1  90. 130.  20  20  50. 90.
06 RFUEL1 110. 150.  20  25   0. 50.
06 RFUEL2   0.  30.  15  65   0. 130.
06 RFUEL2  30.  70.  20  50   0. 110.
06 RFUEL2  70. 110.  20  35   0. 70.
06 RFUEL2 110. 130.  10  15   0. 30.
06 RFUE2R   0.  10.   5   5   0. 10.
06 RFUE2R  70.  90.  10   5   0.  10.
06 RFUE2R   0.  10.   5  10  70.  90.
06 RFUE2R  70.  90.  10  10  70.  90.
06 BACKGR  70. 170.  50  10 150. 170.
06 BACKGR 110. 170.  30  20 130. 150.
06 BACKGR 130. 170.  20  10 110. 130.
06 BACKGR 150. 170.  10  20  70. 110.
10 CBACKG
11 1.0 .5
14 CFUEL1 FUEL1  1.
14 CFUEL2 FUEL2  1.
14 CFUE2R FUEL2R 1.
14 CREFL  REFL   1.
14 CBACKG BLACK  1.
15 CFUEL1 RFUEL1
15 CFUEL2 RFUEL2
15 CFUE2R RFUE2R
15 CREFL  RREFL
15 CBACKG BACKGR
34 ** .8E-4
43 1 5.5 5.5
NOSORT=A.ISO
 0V ISOTXS ISOTXS*IAEA  BNCHMK*     1
 1D      2     6     0     1     1     1     1     1
 2D * 2 GROUP CROSS SECTIONS FOR IAEA BENCHMARK PROBLEM                *
*      * FUEL1  FUEL2  FUEL2R REFL   REFLR  BLACK
 1.00000E+00 0.0
 1.00000E+09 2.20000E+05 1.00000E+07 1.00000E+00 0.0
     0     3     6     9    12    15
 4D  FUEL1 IAEA
 1.00000E+00 3.20000E-11 0.0         0.0         0.0         0.0
     0     0     1     0     0     0     0     0     1     1     0     0
     1     1     2     1     1
 5D  2.22222E-01 8.33333E-01 3.00000E-02 8.00000E-02 1.00000E-02
 3.50000E-02 0.0         4.50000E-02 3.00000E+00 3.00000E+00
 7D  0.0         0.0         2.00000E-02
 4D  FUEL2  IAEA
 1.00000E+00 3.20000E-11 0.0         0.0         0.0         0.0
     0     0     1     0     0     0     0     0     1     1     0     0
     1     1     2     1     1
 5D  2.22222E-01 8.33333E-01 3.00000E-02 8.50000E-02 1.00000E-02
 4.00000E-02 0.0         4.50000E-02 3.00000E+00 3.00000E+00
 7D  0.0         0.0         2.00000E-02
 4D  FUEL2R IAEA
 1.00000E+00 3.20000E-11 0.0         0.0         0.0         0.0
     0     0     1     0     0     0     0     0     1     1     0     0
     1     1     2     1     1
 5D  2.22222E-01 8.33333E-01 3.00000E-02 1.30000E-01 1.00000E-02
 8.50000E-02 0.0         4.50000E-02 3.00000E+00 3.00000E+00
 7D  0.0         0.0         2.00000E-02
 4D  REFL   IAEA
 1.00000E+00 3.20000E-11 0.0         0.0         0.0         0.0
     0     0     0     0     0     0     0     0     1     1     0     0
     1     1     2     1     1
 5D  1.66667E-01 1.11111E+00 4.00000E-02 1.00000E-02 0.0
 1.00000E-02
 7D  0.0         0.0         4.00000E-02
 4D  REFLR  IAEA
 1.00000E+00 3.20000E-11 0.0         0.0         0.0         0.0
     0     0     0     0     0     0     0     0     1     1     0     0
     1     1     2     1     1
 5D  1.66667E-01 1.11111E+00 4.00000E-02 5.50000E-02 0.0
 5.50000E-02
 7D  0.0         0.0         4.00000E-02
 4D  BLACK  IAEA
 1.00000E+00 3.20000E-11 0.0         0.0         0.0         0.0
     0     0     0     0     0     0     0     0     1     1     0     0
     1     1     2     1     1
 5D  1.66667E-01 1.11111E+00 1.00000E+00 1.00000E+00 1.00000E+00
 1.00000E+00
 7D  0.0         0.0         0.0
BLOCK=STP021
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
MODIFY=A.DIF3D
01     IAEA 3D BENCHMARK     10. CM MESH
02 8000 166000
06 0. 0. .01
MODIFY=A.NIP3
01     IAEA 3D BENCHMARK      10. CM MESH
02 0 1 3000 0 1000 0 0 0 0 1
```

Fig. 5.2. Input Data for the IAEA Benchmark Problem Models

```
03  44
04 3 4 3 4 4 4
05 XU .5
05 YU .5
05 ZL .5
05 ZU .5
06 RREFL    0. 170.  0 38   0. 170.
06 RFUEL1   0.  50.  2 36 110. 150.
06 RFUEL1  50.  90.  2 36  90. 130.
06 RFUEL1  90. 110.  2 36  90. 110.
06 RFUEL1  90. 130.  2 36  50.  90.
06 RFUEL1 110. 150.  2 36   0.  50.
06 RFUEL2   0.  30.  2 36   0. 130.
06 RFUEL2  30.  70.  2 36   0. 110.
06 RFUEL2  70. 110.  2 36   0.  70.
06 RFUEL2 110. 130.  2 36   0.  30.
06 RFUE2R   0.  10.  2 36   0.  10.
06 RFUE2R  70.  90.  2 36   0.  10.
06 RFUE2R   0.  10.  2 36  70.  90.
06 RFUE2R  70.  90.  2 36  70.  90.
06 RFUE2R  30.  50. 28 36  30.  50.
06 RREFLR   0.  10. 36 38   0.  10.
06 RREFLR  70.  90. 36 38   0.  10.
06 RREFLR   0.  10. 36 38  70.  90.
06 RREFLR  70.  90. 36 38  70.  90.
06 RREFLR  30.  50. 36 38  30.  50.
06 BACKGR  70. 170.  0 38 150. 170.
06 BACKGR 110. 170.  0 38 130. 150.
06 BACKGR 130. 170.  0 38 110. 130.
06 BACKGR 150. 170.  0 38  70. 110.
10 CBACKG
11 1.0 .5
09 X 17 170.
09 Y 17 170.
09 Z 38 380.
14 CFUEL1 FUEL1  1.
14 CFUEL2 FUEL2  1.
14 CFUE2R FUEL2R 1.
14 CREFL  REFL   1.
14 CREFLR REFLR  1.
14 CBACKG BLACK  1.
15 CFUEL1 RFUEL1
15 CFUEL2 RFUEL2
15 CFUE2R RFUE2R
15 CREFL  RREFL
15 CREFLR RREFLR
15 CBACKG BACKGR
34=DELETE
43=DELETE
```

Fig. 5.2. Input Data for the IAEA Benchmark Problem Models (contd.)

5.4.2 Storage Allocation Routines

The BPOINTER container allocation is done in a FORTRAN subroutine named IGTLCM (with entry point IGTSCM). At individual installations there may be special system routines available which could be called from IGTLCM to borrow space from the system or to return it. Programmers should look at IGTLCM to see if modifications are in order.

5.4.3 TIMER

The subroutine TIMER is a general timing routine specified by the CCCC. The specifications for the subroutine include elapsed central processor time, remaining "limiting" time, elapsed peripheral processor time, current date, user identification, user account, user case identification and wall clock time. Many of these options are installation dependent so that they are not implemented in the export version of TIMER. The options which are not implemented are not required for execution of DIF3D although various timing edits are zeroed in the export version of TIMER. Programmers interested in obtaining proper edits should modify TIMER according to local conventions to implement the desired options.

5.4.4 GNIP4C Graphics

The graphics region map options in the GNIP4C input processor are not operational in the NESC version of DIF3D; they are not crucial to the execution of the code, and graphics systems vary from system to system. An effort was made, however, to make it as simple as possible to implement these options.

1. All graphics calls for the orthogonal geometry maps are made through the subroutine ORTPC2, and all graphics calls for maps of arrays of hexagons are made through HEXPC5. It should be possible to limit code modifications to these two routines.

2. The graphics map routines were coded and checked out for three different graphics systems: CALCOMP, DISPLA and the local Argonne graphics primitives. Code peculiar to CALCOMP and DISPLA were commented out but are identified by comment cards of the form:

```
C**** DISPLA GRAPHICS
        or
C**** CALCOMP GRAPHICS
```

   It should not be hard to reactivate the DISPLA or CALCOMP options.

3. On some systems additional, initialization calls may have to be made.

5.4.5 Random Access I/O Routines DOPC, DRED and DRIT

In the implementation of DOPC that accompanies the NESC package each code block using DOPC initializes it in their respective driver subroutines. On IBM systems DRED (DRIT) call REED (RITE) to perform asynchronous, random access I/O. On CDC 7600 systems, the mass storage routines READMS, WRITMS, OPENMS and CLOSMS are used. On the CRAY-1 FORTRAN '77 I/O statements provide random access capabilities. Installations with asynchronous, random access capabilities superior to those previously mentioned may simply replace DOPC, DRED, DRIT, CRED and CRIT. The latter two routines must be replaced or modified to maintain ECM referencing consistent with any replacement DOPC implementations.

ACKNOWLEDGEMENTS

A number of people have contributed significantly to the programming in the DIF3D code package. C. H. Adams chiefly managed the evolution of the GNIP4C input processor from the FX2 input processor; the broader picture of the evolution of the CCCC routines was also greatly influenced by him. GNIP4C was touched by many others including B. J. Toppel, R. P. Hosteny, Herb Henryson II and several summer students. R. P. Hosteny coded the HMG4C code block. The nodal solution option overlays are the work of R. D. Lawrence. I am indebted to D. R. Ferguson who originally outlined the basic code structure of DIF3D and chose the iteration strategies. Contributions to this report were made by C. H. Adams, H. Henryson II, R. P. Hosteny and B. J. Toppel. Users whose feedback uncovered bugs during the development stages are gratefully acknowledged. A. R. Hinds made several fine tuning suggestions to improve the running times of the inner iteration kernal, SORINV, on the IBM 370/195. Significant CPU time reductions were also achieved on the CDC 7600 with a COMPASS assembler version of SORINV written by F. E. Dunn. For the assistance of L. Rudsinski with the implementation of DIF3D on the CRAY-1 at NCAR, and F. Brinkley and D. McCoy on the CRAY-1 with CTSS at Los Alamos I am indebted. The work of Karen Leffler and Eileen Johnson in typing this report is greatly appreciated.

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Appendix A

ARCSP021 INSTREAM JCL PROCEDURE FOR IBM 370 SYSTEMS

```
//ARCSP021 PROC ATCYL=5,ATDSP='(,DELETE)',ATFLUX='&ATFLUX',
//              ATVOL=,DEST='*',DEST2=F,DMPDEST=F,
//              DMY1CYL=21,DMY2CYL=7,DMY5CYL=4,
//              FDCCYL=20,FLXCYL=1,HALFTRK=6136,
//              ISOCYL=1,ISODSP='(MOD,KEEP)',ISOVOL=,
//              ISOTXS='&ISOTXS',MODEDCB='RECFM=U',
//              MODLIB1='SYS1.DUMMYLIB',
//              MODLIB2='C116.NESC.MODLIB',
//              NACYL=5,NADSP='(,DELETE)',NAFLUX='&NAFLUX',NAVOL=,
//              NHCYL=5,NHDSP='(,DELETE)',NHFLUX='&NHFLUX',NHVOL=,
//              PATH='STP021',
//              POSTLIB='SYS1.DUMMYLIB',PRELIB='SYS1.DUMMYLIB',
//              PSICYL=5,PSUCYL=3,QRTRTRK=3064,REGN=1000K,
//              RTCYL=5,RTDSP='(,DELETE)',RTFLUX='&RTFLUX',
//              RTVOL=,TIMLIM='(600,0)',TWELTRK=1016,
//              SRFCYL=12,
//              UNITS=BATCHDSK,UNITSCR=SASCR,
//              ZONCYL=1
//*
//*    ******************************************************************
//*    *                                                                *
//*    *CATALOGED PROCEDURE FOR 1, 2 OR 3D DIFFUSION CODE DIF3D 3.0    *
//*    *LAST MODIFIED  6/09/83,  PREVIOUSLY MODIFIED  5/16/83          *
//*    *                                                                *
//*    ******************************************************************
//*
//*  ********************************************************************
//*
//*  PARAMETER    DEFAULT VALUE              USAGE                FTNNF001
//*  =========    =============              =====                ========
//*
//*   PATH         STP021           PROGRAM NAME                   EXEC
//*   TIMLIM       (600,0)          STEP TIME LIMIT                EXEC
//*   REGN         1000K            STEP REGION SIZE               EXEC
//*   MODLIB1      SYS1.DUMMYLIB    SECOND STEP LIBRARY            STEPLIB
//*   MODLIB2      C116.NESC.MODLIB NESC SYSTEM LIBRARY            STEPLIB
//*   PRELIB       SYS1.DUMMYLIB    FIRST STEP LIBRARY             STEPLIB
//*   POSTLIB      SYS1.DUMMYLIB    LAST STEP LIBRARY              STEPLIB
//*   DEST         *                OUTPUT DEST. (PRINTER)         06
//*   DEST2        F                OUTPUT DESTINATION FICHE       10
//*   DMPDEST      F                ROUTE DUMP TO FICHE            SYSUDUMP
//*   ATCYL        5                NO. OF CYL. FOR ATFLUX         31
//*   ATDSP        (,DELETE)        DISPOSITION OF ATFLUX          31
//*   ATFLUX       &ATFLUX          DSN FOR DATASET ATFLUX         31
//*   ATVOL        ------           VOLUME FOR ATFLUX              31
//*   ISOCYL       1                NO. CYL. FOR ISOTXS            27
//*   ISODSP       (MOD,KEEP)       DISPOSITION OF ISOTXS          27
//*   ISOTXS       &ISOTXS          DSN FOR DATASET ISOTXS         27
//*   ISOVOL       ------           VOLUME FOR ISOTXS              27
//*   NADSP        (,DELETE)        DISPOSITION OF NAFLUX          24
//*   NAFLUX       &NAFLUX          DSN FOR NAFLUX                 24
//*   NAVOL        ------           VOLUME FOR NAFLUX              24
//*   NHCYL        5                NO. OF CYL. FOR NHFLUX         23
//*   NHDSP        (,DELETE)        DISPOSITION OF NHFLUX          23
//*   NHFLUX       &NHFLUX          DSN FOR NHFLUX                 23
//*   NHVOL        ------           VOLUME FOR NHFLUX              23
//*   RTCYL        5                NO. OF CYL. FOR RTFLUX         30
//*   RTDSP        (,DELETE)        DISPOSITION OF RTFLUX          30
//*   RTFLUX       &RTFLUX          DSN FOR DATASET RTFLUX         30
//*   RTVOL        ------           VOLUME FOR RTFLUX              30
//*   SRFCYL       12               NO. OF CYL. FOR SURF. FLUXES   66,67
//*
//*   THE FOLLOWING FIVE PARAMETERS DEFINE CYLINDER ALLOCATION
//*   AND THE DCB FOR AUXILIARY FLUX, FDCOEF AND ZONMAP DATASETS
//*
//*   FDCCYL       20               NO. OF CYL. FOR FDCOEF DATASET 45
//*   FLXCYL       1                NO. CYL. FOR 1 GROUP FLUX FILES46-49,51,55,
//*   MODEDCB      RECFM=U          DCB FOR MAJOR IO DATASETS      41,52,55,56
//*   PSICYL       5                NO. CYL. FOR FLUX DATASETS     41-42,54
//*   PSUCYL       3                NO. CYL. FOR ADJ. UPSCAT FLUX  43
//*   ZONCYL       1                NO. CYL FOR ZONMAP             52
//*
//*   THE FOLLOWING THREE PARAMETERS DEFINE CYLINDER ALLOCATION
//*   FOR DUMMY FILES WHICH ALLOCATE CONTIGUOUS BLOCKS OF SPACE
//*   TO BE SUBALLOCATED TO VARIOUS SCRATCH DATA SETS.
//*
//*   DMY1CYL      21               NO. OF CYL. FOR FDCOEF, ZONMAP 45,52
//*   DMY2CYL       7               NO. OF CYL. FOR FLUX DATASETS  (41,46,55)
//*                                                                (42,47,56)  (48,51,54)
//*   DMY5CYL       4               NO. OF CYL. FOR FLUX DATASETS  (43,49)
//*
//*   THE FOLLOWING SIX PARAMETERS DEFINE UNIT AND BLKSIZE FOR
//*   A VARIETY OF DATASETS
//*
//*   HALFTRK      6136             HALF TRACK BLOCKING
//*   QRTRTRK      3064             QUARTER TRACK BLOCKING
//*   TWELTRK      1016             TWELFTH TRACK BLOCKING
//*   UNITS        BATCHDSK     -   GENERIC UNIT NAME
//*   UNITSCR      SASCR            GENERIC UNIT NAME
//*
//*  ********************************************************************
//*
//STP021 EXEC PGM=&PATH,TIME=&TIMLIM,REGION=&REGN
//STEPLIB  DD DSN=&PRELIB,DISP=SHR
//         DD DSN=&MODLIB1,DISP=SHR
//         DD DSN=&MODLIB2,DISP=SHR
//         DD DSN=&POSTLIB,DISP=SHR
```

```
//DUMMY1 DD DSN=&&DUMMY1,SPACE=(CYL,(&DMY1CYL,1),,CONTIG),
//             UNIT=&UNITSCR                                          X
//             SHARED BY FDCOEF(45),ZONMAP(52)
//DUMMY2 DD DSN=&&DUMMY2,SPACE=(CYL,(&DMY2CYL,1),,CONTIG),
//             UNIT=(&UNITSCR,SEP=(DUMMY1))                           X
//             SHARED BY PSIOLD(41),PSIGO(55),FRNOLD(46)
//DUMMY3 DD DSN=&&DUMMY3,SPACE=(CYL,(&DMY2CYL,1),,CONTIG),
//             UNIT=(&UNITSCR,SEP=(DUMMY1,DUMMY2))                    X
//             SHARED BY PSINEW(42),PSIGN(56),FRNNEW(47)
//DUMMY4 DD DSN=&&DUMMY4,SPACE=(CYL,(&DMY2CYL,1),,CONTIG),
//             UNIT=(&UNITSCR,SEP=(DUMMY1,DUMMY2,DUMMY3))             X
//             SHARED BY FRNM1(48),SRCNEW(51),FSRC(54)
//DUMMY5 DD DSN=&&DUMMY5,SPACE=(CYL,(&DMY5CYL,1),,CONTIG),
//             UNIT=(&UNITSCR,SEP=(DUMMY1,DUMMY2,DUMMY3,DUMMY4))      X
//             SHARED BY FRNM2(49),PSIUP(43)
//FT05F001 DD DDNAME=SYSIN                                            X
//             BCD INPUT.
//FT06F001 DD SYSOUT=&DEST,DCB=(RECFM=FBA,LRECL=133,BLKSIZE=1596)     X
//             PRINTED OUTPUT.
//FT09F001 DD UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=84,BLKSIZE=&QRTRTRK)              X
//             ARC SYSTEM SPOOLED OUTPUT.
//FT10F001 DD DCB=(RECFM=FBA,LRECL=133,BLKSIZE=1596),SYSOUT=&DEST2    X
//             ALTERNATE PRINT FILE.
//*
//*            DATASETS 11 TO 17 ARE MODULE DEPENDENT BCD DATASETS
//*
//FT11F001 DD DSN=&&ADIF3D,UNIT=&UNITSCR,SPACE=(TRK,(1,5)),
//             DCB=(RECFM=VBS,LRECL=84,BLKSIZE=&TWELTRK)              X
//             1,2 OR 3D DIFFUSION MODULE DEPENDENT BCD DATASET.
//FT12F001 DD DSN=&&ANIP3,UNIT=&UNITSCR,SPACE=(TRK,(4,1)),
//             DCB=(RECFM=VBS,LRECL=84,BLKSIZE=&QRTRTRK)              X
//             THE ARC SYSTEM GENERAL NEUTRONICS BCD DATASET.
//FT13F001 DD DSN=&&AHMG4C,UNIT=&UNITSCR,SPACE=(TRK,(1,0)),
//             DCB=(RECFM=VBS,LRECL=84,BLKSIZE=&TWELTRK)              X
//             CCCC HOMOGENIZATION MODULE DEPENDENT BCD DATASET.
//FT15F001 DD DSN=&&AISO,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=84,BLKSIZE=&QRTRTRK)              X
//             THE ISOTXS BCD DATASET.
//*
//*            DATASETS 18 TO 25 ARE MODULE DEPENDENT BINARY DATASETS.
//*
//FT18F001 DD DSN=&&DIF3D,UNIT=&UNITSCR,SPACE=(TRK,(1,0)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&QRTRTRK)               X
//             1, 2 OR 3D DIFFUSION MODULE DEPENDENT BINARY DATASET.
//FT19F001 DD DSN=&&COMPXS,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             COMPOSITION MACROSCOPIC CROSS-SECTION DATASET.
//FT20F001 DD DSN=&&LABELS,UNIT=&UNITSCR,SPACE=(TRK,(3,0)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&TWELTRK)               X
//             A.NIP3 LABELS AND AREA DEFINITIONS.
//FT22F001 DD DSN=&D3EDIT,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             DIF3D EDITS INTERFACE DATASET.
//FT23F001 DD DSN=&NHFLUX,DISP=&NHDSP,SPACE=(CYL,(&NHCYL,1)),
//             UNIT=&UNITS,VOL=SER=&NHVOL,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             RESTART FILE FOR REAL NODAL HEX CALCULATION.
//FT24F001 DD DSN=&NAFLUX,DISP=&NADSP,SPACE=(CYL,(&NACYL,1)),
//             UNIT=&UNITS,VOL=SER=&NAVOL,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             RESTART FILE FOR ADJOINT NODAL HEX CALCULATION.
//FT25F001 DD DSN=&PKEDIT,UNIT=&UNITSCR,SPACE=(CYL,(1,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             PEAK POWER DENSITY AND FLUX INTERFACE DATASET.
//*
//*            DATASETS 26 TO 40 ARE CCCC INTERFACE FILES.
//*
//FT26F001 DD DSN=&GEODST,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC GEOMETRY DESCRIPTION DATASET.
//FT27F001 DD DSN=&ISOTXS,DISP=&ISODSP,SPACE=(CYL,(&ISOCYL,1)),
//             UNIT=&UNITS,VOL=SER=&ISOVOL,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC NUCLIDE-ORDERED MICROSCOPIC CROSS SECTIONS.
//FT28F001 DD DSN=&NDXSRF,UNIT=&UNITSCR,SPACE=(TRK,(03,0)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC NUCLIDE/CROSS SECTION REFERENCING DATA.
//FT29F001 DD DSN=&ZNATDN,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC ZONE NUCLIDE ATOM DENSITIES.
//FT30F001 DD DSN=&RTFLUX,DISP=&RTDSP,SPACE=(CYL,(&RTCYL,1)),
//             UNIT=&UNITS,VOL=SER=&RTVOL,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC REAL FLUX INTERFACE DATASET.
//FT31F001 DD DSN=&ATFLUX,DISP=&ATDSP,SPACE=(CYL,(&ATCYL,1)),
//             UNIT=&UNITS,VOL=SER=&ATVOL,
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC ADJOINT FLUX INTERFACE DATASET.
//FT32F001 DD DSN=&FIXSRC,UNIT=&UNITS,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC FIXED SOURCE DATASET.
//FT33F001 DD DSN=&RZFLUX,UNIT=&UNITS,SPACE=(TRK,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC ZONE AVERAGED FLUX INTERFACE DATASET.
//FT34F001 DD DSN=&PWDINT,UNIT=&UNITS,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC POWER DENSITY INTERFACE DATASET.
//FT39F001 DD DSN=&SEARCH,UNIT=&UNITSCR,SPACE=(TRK,(03,0)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)               X
//             CCCC CRITICALITY SEARCH DATA.
//*
//*            DATASETS 41 TO 60 ARE SCRATCH DATASETS.
//*
//FT41F001 DD DSN=&&PSIOLD,SUBALLOC=(CYL,(&PSICYL,1),DUMMY2),
//             DCB=&MODEDCB                                           X
//             FLUX ITERATE SCRATCH DATASET.
//FT42F001 DD DSN=&&PSINEW,SUBALLOC=(CYL,(&PSICYL,1),DUMMY3),
```

```
//             DCB=&MODEDCB                                                  X
//             FLUX ITERATE SCRATCH DATASET.
//FT43F001 DD DSN=&&PSIUP,SUBALLOC=(CYL,(&PSUCYL,1),DUMMY5),
//             DCB=&MODEDCB                                                  X
//             AUXILIARY FLUX DATASET FOR ADJOINT UPSCATTER ITERATIONS
//FT45F001 DD DSN=&&FDCOEF,SUBALLOC=(CYL,(&FDCCYL,5),DUMMY1),
//             DCB=&MODEDCB                                                  X
//             FINITE DIFFERENCE COEFFICIENTS SCRATCH DATASET.
//FT46F001 DD DSN=&&FRNOLD,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY2),
//             DCB=&MODEDCB                                                  X
//             FISSION SOURCE SCRATCH DATASET
//FT47F001 DD DSN=&&FRNNEW,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY3),
//             DCB=&MODEDCB                                                  X
//             FISSION SOURCE SCRATCH DATASET
//FT48F001 DD DSN=&&FRNM1,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY4),
//             DCB=&MODEDCB                                                  X
//             FISSION SOURCE SCRATCH DATASET.
//FT49F001 DD DSN=&&FRNM2,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY5),
//             DCB=&MODEDCB                                                  X
//             FISSION SOURCE SCRATCH DATASET.
//FT51F001 DD DSN=&&SRCNEW,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY4),
//             DCB=&MODEDCB                                                  X
//             TOTAL SOURCE SCRATCH DATASET.
//FT52F001 DD DSN=&&ZONMAP,SUBALLOC=(CYL,(&ZONCYL,1),DUMMY1),
//             DCB=&MODEDCB                                                  X
//             ZONE MAP SCRATCH DATASET.
//FT53F001 DD DSN=&&CXSECT,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=&MODEDCB                                                  X
//             COMPOSITION CROSS SECTIONS SCRATCH DATASET.
//FT54F001 DD DSN=&&FSRC,SUBALLOC=(CYL,(&PSICYL,1),DUMMY4),
//             DCB=&MODEDCB                                                  X
//             FIXED SOURCE SCRATCH DATASET.
//FT55F001 DD DSN=&&PSIGO,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY2),
//             DCB=&MODEDCB                                                  X
//             FLUX ITERATE SCRATCH DATASET ONE GROUP.
//FT56F001 DD DSN=&&PSIGN,SUBALLOC=(CYL,(&FLXCYL,1),DUMMY3),
//             DCB=&MODEDCB                                                  X
//             FLUX ITERATE SCRATCH DATASET ONE GROUP.
//*
//*            DATASETS 66 TO 71 ARE SCRATCH DATASETS
//*
//FT66F001 DD DSN=&SCR001,UNIT=&UNITSCR,SPACE=(CYL,(&SRFCYL,2)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             SCRATCH FILE 1.
//FT67F001 DD DSN=&SCR002,UNIT=&UNITSCR,SPACE=(CYL,(&SRFCYL,2)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             SCRATCH FILE 2.
//FT68F001 DD DSN=&SCR003,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             SCRATCH FILE 3.
//FT69F001 DD DSN=&SCR004,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             SCRATCH FILE 4.
//FT70F001 DD DSN=&SCR005,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             SCRATCH FILE 5.
//FT71F001 DD DSN=&SCR006,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             SCRATCH FILE 6.
//*
//*            DATASETS 76 TO 80 ARE UDOIT INTERFACE DATASETS
//*
//FT76F001 DD DSN=&UDOIT1,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             UDOIT INTERFACE FILE VERSION 1.
//FT77F001 DD DSN=&UDOIT2,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             UDOIT INTERFACE FILE VERSION 2.
//FT78F001 DD DSN=&UDOIT3,UNIT=&UNITSCR,SPACE=(CYL,(01,1)),
//             DCB=(RECFM=VBS,LRECL=X,BLKSIZE=&HALFTRK)                      X
//             UDOIT INTERFACE FILE VERSION 3.
//FT80F001 DD DSN=&AUDOIT,UNIT=&UNITSCR,SPACE=(TRK,(3,1)),
//             DCB=(RECFM=VBS,LRECL=84,BLKSIZE=&QRTRTRK)                     X
//             BCD INPUT DATASET FOR UDOIT MODULES.
//SYSUDUMP DD SYSOUT=&DMPDEST                                                X
//             SYSTEM DUMP DATASET FOR ABNORMAL JOB TERMINATION.
//         PEND
```

Appendix B

DIF3D BCD INPUT FILE DESCRIPTIONS

B.1 A.DIF3D

```
C*****************************************************************************
C                                                                             -
C                        REVISED 12/15/82                                     -
C                                                                             -
CF          A.DIF3D                                                           -
CE          ONE-, TWO-, AND THREE-DIMENSIONAL DIFFUSION THEORY                -
CE          MODULE-DEPENDENT BCD INPUT                                        -
C                                                                             -
CN                       THIS BCD DATASET MAY BE WRITTEN EITHER              -
CN                       IN FREE FORMAT (UNFORM=A.DIF3D) OR                  -
CN                       ACCORDING TO THE FORMATS SPECIFIED FOR EACH         -
CN                       CARD TYPE (DATASET=A.D F3D).                        -
CN                                                                           -
CN                       COLUMNS 1-2 MUST CONTAIN THE CARD TYPE NUMBER.      -
CN                                                                           -
CN                       A BLANK OR ZERO FIELD GIVES THE DEFAULT OPTION      -
CN                       INDICATED.                                          -
CN                                                                           -
CN                       NON-DEFAULTED DATA ITEMS ON THE A.DIF3D             -
CN                       DATA SET ALWAYS OVERRIDE THE CORRESPONDING          -
CN                       DATA ON THE RESTART DATA SET DIF3D.                 -
C                                                                             -
C*****************************************************************************

C-----------------------------------------------------------------------------
CR          PROBLEM TITLE (TYPE 01)                                          -
C                                                                            -
CL     FORMAT-----(I2,4X,11A6)                                               -
C                                                                            -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                      -
CD     =======  ==========================================================  -
CD     1-2      01                                                          -
CD                                                                           -
CD     7-72     ANY ALPHANUMERIC CHARACTERS (1 CARD ONLY).                  -
C                                                                            -
C-----------------------------------------------------------------------------

C-----------------------------------------------------------------------------
CR          STORAGE AND DUMP SPECIFICATIONS (TYPE 02)                        -
C                                                                            -
CL          FORMAT-----(I2,4X,3I6)                                           -
C                                                                            -
CD          COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                 -
CD     =======  ==========================================================  -
CD     1-2      02                                                          -
CD                                                                           -
CD     7-12     POINTR CONTAINER ARRAY SIZE IN FAST CORE MEMORY (FCM)       -
CD              IN REAL*8 WORDS (DEFAULT=10000).                            -
CD                                                                           -
CD     13-18    POINTR CONTAINER ARRAY SIZE IN EXTENDED CORE                -
CD              MEMORY (ECM) IN REAL*8 WORDS (DEFAULT=30000).               -
CD                                                                           -
CD     19-24    POINTR DEBUGGING EDIT.                                      -
CD              0...NO DEBUGGING PRINTOUT (DEFAULT).                        -
CD              1...DEBUGGING DUMP PRINTOUT.                                -
CD              2...DEBUGGING TRACE PRINTOUT.                               -
CD              3...BOTH DUMP AND TRACE PRINTOUT.                           -
C                                                                            -
C-----------------------------------------------------------------------------

C-----------------------------------------------------------------------------
CR          PROBLEM CONTROL PARAMETERS (TYPE 03)                             -
C                                                                            -
CL     FORMAT-----(I2,4X,11I6)                                               -
C                                                                            -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                      -
CD     =======  ==========================================================  -
CD     1-2      03                                                          -
CD                                                                           -
CD     7-12     PROBLEM TYPE.                                               -
CD              0...K-EFFECTIVE PROBLEM (DEFAULT).                          -
CD              1...FIXED SOURCE PROBLEM.                                   -
CD                                                                           -
CD     13-18    SOLUTION TYPE.                                              -
CD              0...REAL SOLUTION (DEFAULT).                                -
CD              1...ADJOINT SOLUTION.                                       -
CD              2...BOTH REAL AND ADJOINT SOLUTION.                         -
CD                                                                           -
CD     19-24    CHEBYSHEV ACCELERATION OF OUTER ITERATIONS.                 -
CD              0...YES, ACCELERATE THE OUTER ITERATIONS (DEFAULT).         -
CD              1...NO ACCELERATION.                                        -
CD                                                                           -
CD     25-30    MINIMUM PLANE-BLOCK (RECORD) SIZE IN REAL*8 WORDS FOR       -
CD              I/O TRANSFER IN THE CONCURRENT INNER ITERATION              -
CD              STRATEGY. THE DEFAULT (=4500) IS HIGHLY RECOMMENDED.        -
CD                                                                           -
CD     31-36    OUTER ITERATION CONTROL.                                    -
CD              -3...BYPASS DIF3D MODULE.                                   -
CD              -2...CALCULATE DATA MANAGEMENT PARAMETERS AND PERFORM       -
CD                   NEUTRONICS EDITS ONLY.                                 -
CD              -1...CALCULATE DATA MANAGEMENT PARAMETERS, CALCULATE        -
CD                   OVERRELAXATION FACTORS AND PERFORM NEUTRONICS           -
```

```
CD                EDITS ONLY.                                              -
CD          .GE.0...MAXIMUM NUMBER OF OUTER ITERATIONS (DEFAULT=30).       -
CD                                                                         -
CD   37-42    RESTART FLAG.                                                -
CD            0...THIS IS NOT A RESTART (DEFAULT).                         -
CD            1...THIS IS A RESTART PROBLEM.                               -
CD                                                                         -
CD   43-48    JOB TIME LIMIT, MAXIMUM (CP AND PP(OR WAIT)) PROCESSOR       -
CD            SECONDS (DEFAULT=1000000000).                                -
CD                                                                         -
CD   49-54    NUMBER OF UPSCATTER ITERATIONS PER OUTER ITERATION            -
CD            (DEFAULT=5).  PERTINENT TO UPSCATTER PROBLEMS ONLY.          -
CD                                                                         -
CD   55-60    CONCURRENT ITERATION EFFICIENCY OPTION.                       -
CD            0...PERFORM THE ESTIMATED NO. OF INNER ITERATIONS FOR         -
CD                EACH GROUP.                                              -
CD            1...AVOID THE LAST PASS OF INNER ITERATIONS IN THOSE          -
CD                GROUPS FOR WHICH THE NO. OF ITERATIONS IN THE LAST       -
CD                PASS ARE LESS THAN A CODE DEPENDENT THRESHOLD.            -
CD                                                                         -
CD   61-66    ACCELERATION OF OPTIMUM OVERRELAXATION FACTOR                 -
CD            CALCULATION.                                                 -
CD            0...NO ACCELERATION (DEFAULT).                               -
CD            1...ASYMPTOTIC SOURCE EXTRAPOLATION OF POWER ITERATIONS-     -
CD                USED TO ESTIMATE THE SPECTRAL RADIUS OF EACH INNER       -
CD                (WITHIN GROUP) ITERATION MATRIX.                         -
CD   67-72    OPTIMUM OVERRELAXATION FACTOR ESTIMATION ITERATION            -
CD            CONTROL. THE DEFAULT (=50) IS STRONGLY RECOMMENDED.          -
C                                                                          -
CN            THE MAXIMUM NUMBER OF OUTER ITERATIONS SENTINEL              -
CN            SPECIFIES THE NUMBER OF OUTERS THAT CAN BE PERFORMED         -
CN            (COLS. 31-36) EACH TIME THE DIF3D MODULE IS INVOKED.         -
CN                                                                         -
CN            THE DIF3D TERMINATION PROCEDURE WILL ALWAYS:                 -
CN                 1...(RE)WRITE THE APPROPRIATE FLUX FILES                -
CN                    (RTFLUX OR ATFLUX).                                  -
CN                 2...(RE)WRITE THE RESTART FILE DIF3D.                   -
CN            TO FACILITATE AUTOMATIC RESTART, THE RESTART FLAG            -
CN            ON THE DIF3D RESTART CONTROL FILE WILL BE TURNED ON          -
CN            AUTOMATICALLY UPON DETECTION OF:                             -
CN                 1...MAXIMUM NUMBER OF OUTER ITERATIONS.                 -
CN                 2...TIME LIMIT.                                         -
CN                                                                         -
CN                                                                         -
CN            TO RESTART THE FLUX CALCULATION:                             -
CN            EITHER                                                       -
CN                                                                         -
CN                PROVIDE THE RESTART DATA SET DIF3D AND                   -
CN                THE APPROPRIATE FLUX DATA SET (RTFLUX OR ATFLUX)         -
CN                AND SPECIFY THEM UNDER "BLOCK=OLD" IN THE BCD            -
CN                INPUT DATA                                               -
CN            OR                                                           -
CN                 1...SET THE RESTART FLAG (COLS. 37-42) TO 1 ON          -
CN                    THE TYPE 03 CARD. THIS PERMITS IMMEDIATE             -
CN                    RESUMPTION OF OUTER ITERATION ACCELERATION.          -
CN                 2...INCLUDE THE LATEST K-EFFECTIVE ESTIMATE             -
CN                    (COLS. 13-24) AND THE DOMINANCE RATIO                -
CN                    ESTIMATE ON THE TYPE 06 CARD (COLS. 61-72).          -
CN                 3...INCLUDE THE OPTIMUM OVERRELAXATION FACTORS          -
CN                    FOR EACH GROUP (TYPE 07 CARD).                       -
CN                 4...PROVIDE THE APPROPRIATE FLUX DATA SET (RTFLUX       -
CN                    OR ATFLUX) AND SPECIFY IT UNDER "BLOCK=OLD"           -
CN                    IN THE BCD INPUT DATA.                               -
CN                                                                         -
CN            A NON-ZERO TIME LIMIT (COLS. 43-48) OVERRIDES                -
CN            THE ACTUAL TIME LIMIT DETERMINED INTERNALLY                  -
CN            BY SYSTEM ROUTINES IN THE ANL AND LBL PRODUCTION             -
CN            IMPLEMENTATIONS                                              -
CN                                                                         -
CN            THE TIME LIMIT PARAMETER (COLS. 43-48) IS PERTINENT          -
CN            TO EACH ENTRY TO THE DIF3D MODULE.                           -
CN                                                                         -
CN            IT IS RECOMMENDED THAT AN ODD NUMBER OF UPSCATTER            -
CN            ITERATIONS BE SPECIFIED (COLS. 49-54) TO AVOID               -
CN            ADDITIONAL I/O OVERHEAD.                                     -
CN                                                                         -
CN            THE USER IS CAUTIONED TO MONITOR THE POINT-WISE              -
CN            FISSION SOURCE CONVERGENCE TO ENSURE THAT MONOTONIC          -
CN            CONVERGENCE IS OBTAINED WHEN THE EFFICIENCY OPTION           -
CN            (COLS. 55-60) IS ACTIVATED.                                  -
CN                                                                         -
CN            THE OPTIMUM OVERRELAXATION FACTOR ACCELERATION OPTION        -
CN            IS PRIMARILY INTENDED FOR PROBLEMS KNOWN TO HAVE HIGH        -
CN            (>1.8) OPTIMUM OVERRELAXATION FACTORS.                       -
CN                                                                         -
CN            ITERATION CONTROL (COLS. 67-72) OF THE OPTIMUM               -
CN            OVERRELAXATION FACTOR ESTIMATION IS PRIMARILY INTENDED -     -
CN            FOR USE IN CONJUNCTION WITH THE ASYMPTOTIC ACCELERATION-     -
CN            OPTION (COLS. 61-66).                                        -
C                                                                          -
C--------------------------------------------------------------------------

C--------------------------------------------------------------------------
CR          EDIT OPTIONS (TYPE 04)                                         -
C                                                                          -
CL    FORMAT-----(I2,4X,1016)                                              -
C                                                                          -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                     -
CD    =======  ------------------------------------------------------------
CD    1-2      04                                                          -
CD                                                                         -
CD    7-12     PROBLEM DESCRIPTION EDIT (IN ADDITION TO USER INPUT         -
CD             SPECIFICATIONS WHICH ARE ALWAYS EDITED.                     -
CD             0...NO EDITS (DEFAULT).                                     -
CD             1...PRINT EDITS.                                            -
CD             2...WRITE EDITS TO AUXILIARY OUTPUT FILE.                   -
CD             3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
```

```
CD                                                                      -
CD   13-18   GEOMETRY (REGION TO MESH INTERVAL) MAP EDIT.               -
CD           0...NO EDITS (DEFAULT).                                    -
CD           1...PRINT EDITS.                                           -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.                  -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                      -
CD   19-24   GEOMETRY (ZONE TO MESH INTERVAL) MAP EDIT.                 -
CD           0...NO EDITS (DEFAULT).                                    -
CD           1...PRINT EDITS.                                           -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.                  -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                      -
CD   25-30   MACROSCOPIC CROSS SECTION EDIT.                           -
CD           ENTER TWO DIGIT NUMBER SP WHERE                            -
CD                                                                      -
CD           S CONTROLS THE SCATTERING AND PRINCIPAL CROSS SECTIONS -
CD           P CONTROLS THE PRINCIPAL CROSS SECTIONS EDIT ONLY.      -
CD                                                                      -
CD           THE INTEGERS S AND P SHOULD BE ASSIGNED ONE OF THE     -
CD           FOLLOWING VALUES (LEADING ZEROES ARE IRRELEVANT).      -
CD           0...NO EDITS (DEFAULT).                                -
CD           1...PRINT EDITS.                                       -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.              -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                  -
CD   31-36   BALANCE EDITS                                          -
CD           ENTER 3 DIGIT NUMBER GBR WHERE                         -
CD                                                                  -
CD           G CONTROLS GROUP BALANCE EDITS INTEGRATED OVER THE     -
CD           REACTOR                                                -
CD           B CONTROLS REGION BALANCE EDIT BY GROUP                -
CD           R CONTROLS REGION BALANCE EDIT TOTALS                  -
CD             (INCLUDING NET PRODUCTION AND ENERGY MEDIANS)        -
CD                                                                  -
CD           THE INTEGERS G, B, AND R SHOULD BE ASSIGNED ONE OF THE -
CD           FOLLOWING VALUES (LEADING ZEROES ARE IRRELEVANT)       -
CD           0...NO EDITS (DEFAULT).                                -
CD           1...PRINT EDITS.                                       -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.              -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                  -
CD   37-42   POWER EDITS                                            -
CD           ENTER 2 DIGIT NUMBER RM WHERE                          -
CD                                                                  -
CD           R CONTROLS REGION POWER AND AVERAGE POWER DENSITY EDITS-
CD           M CONTROLS POWER DENSITY BY MESH INTERVAL EDIT (PWDINT)-
CD                                                                  -
CD           THE INTEGERS R AND M SHOULD BE ASSIGNED                -
CD           ONE OF THE FOLLOWING VALUES (LEADING ZEROES ARE        -
CD           IRRELEVANT)                                            -
CD           0...NO EDITS (DEFAULT).                                -
CD           1...PRINT EDITS.                                       -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.              -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                  -
CD   43-48   FLUX EDITS                                             -
CD           ENTER 3 DIGIT INTEGER RMB WHERE                        -
CD                                                                  -
CD           R CONTROLS FLUX EDIT BY REGION AND GROUP               -
CD             INCLUDING GROUP AND REGION TOTALS                    -
CD           M CONTROLS TOTAL (GROUP INTEGRATED) FLUX EDIT          -
CD             BY MESH INTERVAL                                     -
CD           B CONTROLS TOTAL FLUX EDIT BY MESH INTERVAL AND GROUP  -
CD             (RTFLUX OR ATFLUX)                                   -
CD                                                                  -
CD           THE INTEGERS R, M, AND B SHOULD BE ASSIGNED            -
CD           ONE OF THE FOLLOWING VALUES (LEADING ZEROES ARE        -
CD           IRRELEVANT)                                            -
CD           0...NO EDITS (DEFAULT).                                -
CD           1...PRINT EDITS.                                       -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.              -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                  -
CD   49-54   ZONE AVERAGED (REAL) FLUX EDIT.                        -
CD           0...NO EDITS (DEFAULT).                                -
CD           1...PRINT EDITS.                                       -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.              -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                  -
CD   55-60   REGION AVERAGED FLUX EDIT.                             -
CD           0...NO EDITS (DEFAULT).                                -
CD           1...PRINT EDITS.                                       -
CD           2...WRITE EDITS TO AUXILIARY OUTPUT FILE.              -
CD           3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                  -
CD   61-66   STANDARD INTERFACE FILES TO BE WRITTEN IN ADDITION     -
CD           TO RTFLUX AND/OR ATFLUX.                               -
CD           0...NONE (DEFAULT).                                    -
CD           1...WRITE PWDINT.                                      -
CD           2...WRITE RZFLUX.                                      -
CD           3...WRITE BOTH PWDINT AND RZFLUX.                      -
CD                                                                  -
CD   67-72   MASTER DIF3D EDIT SENTINEL DURING CRITICALITY SEARCHES -
CD          -1...SUPPRESS ALL DIF3D EDITS EXCEPT THE ITERATION      -
CD              HISTORY AND ERROR DIAGNOSTICS                       -
CD           0...EDIT INPUT DATA ON 1ST SEARCH PASS, OUTPUT         -
CD              INTEGRALS UPON CONVERGENCE OR UPON ACHIEVING THE    -
CD              MAXIMUM SEARCH PASS LIMIT.                          -
CD           N...ALSO INVOKE SPECIFIED DIF3D EDITS EVERY N-TH       -
CD              SEARCH PASS.                                        -
C                                                                   -
CN           MULTI-DIGIT EDIT SPECIFICATION EXAMPLES.               -
CN                                                                  -
CN           ENTERING THE INTEGER 201 IN COLUMNS 31-36 YIELDS       -
CN           THE GROUP BALANCE EDIT ON THE AUXILIARY FILE AND       -
CN           THE REGION BALANCE EDIT ON THE PRIMARY PRINT FILE.     -
CN                                                                  -
```

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CN              ENTERING THE INTEGER 30 IN COLUMNS 31-36 YIELDS       -
CN              THE REGION BALANCE EDIT BY GROUP ON BOTH THE PRINT AND -
CN              THE AUXILIARY OUTPUT FILES.                           -
C                                                                     -
C---------------------------------------------------------------------
```

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C---------------------------------------------------------------------
CR          CONVERGENCE CRITERIA (TYPE 05)                            -
C                                                                     -
CL     FORMAT---  --(I2,10X,3E12.5)                                   -
C                                                                     -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY               -
CD     =======  ==========================================================-
CD     1-2      05                                                    -
CD                                                                    -
CD     13-24    EIGENVALUE CONVERGENCE CRITERION FOR STEADY STATE     -
CD              CALCULATION (DEFAULT VALUE = 1.0E-7 IS RECOMMENDED).  -
CD                                                                    -
CD     25-36    POINTWISE FISSION SOURCE CONVERGENCE CRITERION        -
CD              FOR STEADY STATE SHAPE CALCULATION                    -
CD              (DEFAULT VALUE = 1.0E-5 IS RECOMMENDED).              -
CD                                                                    -
CD     37-48    AVERAGE FISSION SOURCE CONVERGENCE CRITERION          -
CD              FOR STEADY STATE SHAPE CALCULATION                    -
CD              (DEFAULT VALUE = 1.0E-5 IS RECOMMENDED).              -
C                                                                     -
CN              IN UPSCATTERING PROBLEMS IT IS RECOMMENDED THAT       -
CN              THE EIGENVALUE CONVERGENCE CRITERION (COLS. 13-24)    -
CN              BE .1 TIMES THE POINTWISE FISSION SOURCE CONVERGENCE  -
CN              CRITERION (COLS. 25-36).                              -
C                                                                     -
C---------------------------------------------------------------------
```

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C---------------------------------------------------------------------
CR          OTHER FLOATING POINT DATA (TYPE 06)                       -
C                                                                     -
CL     FORMAT-------(I2,10X,5E12.5)                                   -
C                                                                     -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY               -
CD     =======  ==========================================================-
CD     1-2      06                                                    -
CD                                                                    -
CD     13-24    K-EFFECTIVE OF REACTOR (DEFAULT IS OBTAINED FROM      -
CD              THE APPROPRIATE RTFLUX OR ATFLUX FILE, IF PRESENT.    -
CD              OTHERWISE DEFAULT = 1.0).                             -
CD                                                                    -
CD     25-36    ANY POINTWISE FISSION SOURCE WILL BE NEGLECTED IN THE -
CD              POINTWISE FISSION SOURCE CONVERGENCE TEST IF IT IS     -
CD              LESS THAN THIS FACTOR TIMES THE R.M.S. FISSION        -
CD              SOURCE (DEFAULT VALUE = .001 IS RECOMMENDED).         -
CD                                                                    -
CD     37-48    ERROR REDUCTION FACTOR TO BE ACHIEVED BY EACH SERIES  -
CD              OF INNER ITERATIONS FOR EACH GROUP DURING A SHAPE     -
CD              CALCULATION - STRONGLY RECOMMENDED THAT THE DEFAULT   -
CD              VALUE OF (.04) BE USED.                               -
CD                                                                    -
CD     49-60    STEADY STATE REACTOR POWER (WATTS). (DEFAULT = 1.0).  -
CD                                                                    -
CD     61-72    DOMINANCE RATIO (FOR RESTART JOBS ONLY).              -
C                                                                     -
CN              K-EFFECTIVE SPECIFICATIONS (COLS. 13-24):             -
CN                   1...FOR K-EFFECTIVE PROBLEMS, SUPPLY ESTIMATED   -
CN                       K-EFFECTIVE OF REACTOR.                      -
CN                   2...FOR RESTARTED K-EFFECTIVE PROBLEMS, SUPPLY   -
CN                       LATEST K-EFFECTIVE ESTIMATE SUPPLIED ON THE  -
CN                       ITERATION HISTORY EDIT.                      -
CN                   3...FOR SOURCE PROBLEMS, SUPPLY K-EFFECTIVE OF   -
CN                       THE REACTOR.                                 -
CN              DEFAULT IS OBTAINED FROM THE APPROPRIATE RTFLUX OR     -
CN              ATFLUX FILE, IF PRESENT.  OTHERWISE DEFAULT=1.0 .      -
C                                                                     -
CN              NON-MONOTONIC POINTWISE FISSION SOURCE CONVERGENCE     -
CN              IS USUALLY INDICATIVE OF THE NEED TO TIGHTEN THE ERROR -
CN              REDUCTION FACTOR(COLS. 37-48).  THIS IS FREQUENTLY TRUE-
CN              IN TRIANGULAR GEOMETRY PROBLEMS WHERE A VALUE OF .01 IS-
CN              USUALLY SUFFICIENT TO OBTAIN MONOTONIC CONVERGENCE.    -
C---------------------------------------------------------------------
```

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C---------------------------------------------------------------------
CR          OPTIMUM OVERRELAXATION FACTORS (TYPE 07)                  -
C                                                                     -
CL     FORMAT-----(I2,10X,5E12.5)                                     -
C                                                                     -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY               -
CD     =======  ==========================================================-
CD     1-2      07                                                    -
CD                                                                    -
CD     13-24    OPTIMUM OVERRELAXATION FACTOR FOR GROUP 1.            -
CD                                                                    -
CD     25-36    OPTIMUM OVERRELAXATION FACTOR FOR GROUP 2.            -
CD                                                                    -
CD     37-48    OPTIMUM OVERRELAXATION FACTOR FOR GROUP 3.            -
CD                                                                    -
CD     49-60    OPTIMUM OVERRELAXATION FACTOR FOR GROUP 4.            -
CD                                                                    -
CD     61-72    OPTIMUM OVERRELAXATION FACTOR FOR GROUP 5.            -
C                                                                     -
CN              REPEAT 5 VALUES PER CARD FOR AS MANY TYPE 07 CARDS    -
CN              AS ARE NEEDED.                                        -
CN                                                                    -
CN              THE OPTIMUM OVERRELAXATION FACTORS ARE NORMALLY       -
CN              OBTAINED FROM THE RESTART INSTRUCTIONS PRINTED        -
CN              IMMEDIATELY AFTER THE DIF3D ITERATION HISTORY EDIT.   -
CN              IN THE RESTART INSTRUCTIONS, THE FACTORS ARE ALWAYS    -
CN              EDITTED IN THE --REAL PROBLEM-- ORDERING AND SHOULD BE -
```

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CN              ENTERED ON THE TYPE 07 CARD --EXACTLY-- AS EDITTED      -
CN              IN THE RESTART INSTRUCTIONS.                            -
CN                                                                      -
CN              THE PERMISSIBLE FACTOR RANGE IS BOUNDED BY 1.0 AND 2.0  -
CN              INCLUSIVE. A ZERO OR BLANK FACTOR ENTRY DEFAULTS        -
CN              TO 1.0. FACTORS ARE COMPUTED FOR THOSE GROUPS HAVING    -
CN              A FACTOR OF 1.0; FACTORS GREATER THAN 1.0 ARE NOT       -
CN              RECOMPUTED.                                             -
CN                                                                      -
CN              TYPE 07 CARDS ARE PRIMARILY INTENDED FOR RESTART JOBS   -
CN              ONLY (STRONGLY RECOMMENDED).                            -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          NEAR CRITICAL SOURCE PROBLEM ASYMPTOTIC EXTRAPOLATION       -
CR          PARAMETERS (TYPE 08)                                        -
C                                                                       -
CC          ***** WARNING...SELECT THIS OPTION ONLY IF THE  *****       -
CC          ***** ASYMPTOTIC EXTRAPOLATION IS REQUIRED FOR  *****       -
CC          ***** THIS PROBLEM.                            *****       -
C                                                                       -
CL      FORMAT-----(I2,4X,I6,E12.5)                                     -
C                                                                       -
CD      COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD      =======  ==========================================================-
CD      1-2      08                                                     -
CD                                                                      -
CD      7-12     NUMBER OF OUTER (POWER) ITERATIONS PERFORMED PRIOR TO  -
CD               ASYMPTOTIC EXTRAPOLATION OF NEAR CRITICAL SOURCE       -
CD               PROBLEM (DEFAULT=5).                                   -
CD                                                                      -
CD      13-24    EIGENVALUE OF THE HOMOGENEOUS PROBLEM CORRESPONDING    -
CD               TO THE NEAR CRITICAL SOURCE PROBLEM. THIS EIGENVALUE   -
CD               MUST BE LESS THAN ONE.                                 -
CD                                                                      -
CD      25-30    INITIAL FLUX GUESS SENTINEL.                           -
CD               0...FLAT FLUX GUESS=1.0 (DEFAULT)                      -
CD               1...FLAT FLUX GUESS=0.0                                -
C                                                                       -
CN              THE TYPE 08 CARD IS REQUIRED TO ACTIVATE AN ALTERNATE   -
CN              SPECIAL ACCELERATION SCHEME FOR NEAR CRITICAL           -
CN              SOURCE PROBLEMS.                                        -
CN                                                                      -
CN              IF COLS. 13-24 ARE ZERO OR BLANK, THE HOMOGENEOUS       -
CN              PROBLEM EIGENVALUE WILL BE ESTIMATED. IN THIS CASE, IT  -
CN              IS RECOMMENDED TO INCREASE THE NUMBER OF ITERATIONS IN  -
CN              COLS. 7-12 TO AT LEAST 10.                              -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SN TRANSPORT OPTIONS (TYPE 09)                              -
C                                                                       -
CL      FORMAT-----(I2,4X,2I6,6X,E12.4)                                 -
C                                                                       -
CD      COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD      =======  ==========================================================-
CD      1-2      09                                                     -
CD                                                                      -
CD      7-12     SN ORDER.                                              -
CD                                                                      -
CD      13-18    MAXIMUM ALLOWED NUMBER OF LINE SWEEPS PER LINE PER     -
CD               INNER ITERATION (DEFAULT=10).                          -
CD                                                                      -
CD      25-36    LINE SWEEP CONVERGENCE CRITERION (DEFAULT=1.0E-4).     -
C                                                                       -
CN              TO INVOKE THE DIF3D TRANSPORT OPTION, THE TYPE 09 CARD  -
CN              MUST BE PRESENT WITH A NONZERO SN ORDER. FOR THE TIME   -
CN              BEING, USERS MUST ALSO CONTINUE TO 'PRELIB' TO          -
CN              DATASET 'C116.B99983.MODLIB' TO INVOKE THIS OPTION.     -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          PARAMETERS FOR NODAL HEXAGONAL GEOMETRY OPTION (TYPE 10)    -
C                                                                       -
CL      FORMAT-----(I2,4X,5I6)                                          -
C                                                                       -
CD      COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD      =======  ==========================================================-
CD      1-2      10                                                     -
CD                                                                      -
CD      7-12     ORDER OF NODAL APPROXIMATION IN HEX-PLANE.             -
CD               2...NH2 APPROXIMATION.                                 -
CD               3...NH3 APPROXIMATION.                                 -
CD               4...NH4 APPROXIMATION (DEFAULT).                       -
CD                                                                      -
CD      13-18    ORDER OF NODAL APPROXIMATION IN Z-DIRECTION.           -
CD               2...QUADRATIC APPROXIMATION.                           -
CD               3...CUBIC APPROXIMATION (DEFAULT).                     -
CD                                                                      -
CD      19-24    COARSE-MESH REBALANCE ACCELERATION CONTROL.            -
CD              -1...NO COARSE-MESH REBALANCE ACCELERATION.             -
CD          .GE.0...NUMBER OF COARSE-MESH REBALANCE ITERATIONS PER      -
CD                  OUTER ITERATION (DEFAULT=2).                       -
CD                                                                      -
CD      25-30    ASYMPTOTIC SOURCE EXTRAPOLATION OF OUTER ITERATIONS.   -
CD               0...APPLY ASYMPTOTIC SOURCE EXTRAPOLATION TO OUTER     -
CD                   ITERATIONS (DEFAULT).                              -
CD               1...NO ASYMPTOTIC SOURCE EXTRAPOLATION.                -
CD                                                                      -
CD      31-36    NUMBER OF AXIAL PARTIAL CURRENT SWEEPS PER GROUP       -
CD               PER OUTER ITERATION (DEFAULT=2).                       -
C                                                                       -
CN              THE TYPE 10 CARD IS PERTINENT ONLY WHEN THE NODAL       -
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CN              HEXAGONAL GEOMETRY OPTION (A.NIP3 TYPE 03 CARD          -
CN              GEOMETRY-TYPE SENTINEL VALUES BETWEEN 110 AND 128)      -
CN              IS SPECIFIED.                                           -
CN                                                                      -
CN              IT IS RECOMMENDED THAT THE DEFAULT VALUES FOR THE       -
CN              ORDER OF THE NODAL APPROXIMATION IN THE HEX-PLANE       -
CN              (COLS. 7-12) AND FOR THE ORDER OF THE NODAL APPROXI-    -
CN              MATION IN THE Z-DIRECTION (COLS. 13-18) BE SPECIFIED.   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          AXIAL COARSE-MESH REBALANCE BOUNDARIES FOR NODAL            -
CR          HEXAGONAL GEOMETRY OPTION (TYPE 11)                         -
C                                                                       -
CL    FORMAT------(I2,10X,3(I6,E12.5))                                  -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      11                                                       -
CD                                                                      -
CD    13-18    NUMBER OF AXIAL COARSE-MESH REBALANCE INTERVALS.         -
CD                                                                      -
CD    19-30    UPPER Z-COORDINATE.                                      -
CD                                                                      -
CD    31-36    NUMBER OF AXIAL COARSE-MESH REBALANCE INTERVALS.         -
CD                                                                      -
CD    37-48    UPPER Z-COORDINATE.                                      -
CD                                                                      -
CD    49-54    NUMBER OF AXIAL COARSE-MESH REBALANCE INTERVALS.         -
CD                                                                      -
CD    55-66    UPPER Z-COORDINATE.                                      -
C                                                                       -
CN              THE TYPE 11 CARD IS PERTINENT ONLY WHEN THE THREE-      -
CN              DIMENSIONAL NODAL HEXAGONAL GEOMETRY OPTION (A.NIP3     -
CN              TYPE 03 CARD GEOMETRY-TYPE SENTINEL VALUES BETWEEN      -
CN              120 AND 128) IS SPECIFIED.                              -
CN                                                                      -
CN              IF NO TYPE 11 CARDS ARE PRESENT, THE AXIAL COARSE-MESH  -
CN              REBALANCE INTERVALS ARE DEFINED BY THE Z-COORDINATE     -
CN              VALUES SPECIFIED ON A.NIP3 CARD 09.                     -
CN                                                                      -
CN              BOUNDARIES ARE SPECIFIED VIA NUMBER PAIRS.              -
CN              EACH NUMBER PAIR IS OF THE FORM (N(I), Z(I)). THERE     -
CN              ARE N(I) AXIAL COARSE-MESH REBALANCE INTERVALS BETWEEN  -
CN              Z(I-1) AND Z(I), WHERE Z(0) IS THE LOWER REACTOR        -
CN              BOUNDARY IN THE Z-DIRECTION. NUMBER PAIRS MUST BE       -
CN              GIVEN IN ORDER OF INCREASING MESH COORDINATES. ALL      -
CN              AXIAL COARSE-MESH REBALANCE BOUNDARIES MUST COINCIDE    -
CN              WITH THE MESH LINES WHICH BOUND MESH INTERVALS.         -
C                                                                       -
C-----------------------------------------------------------------------
CEOF
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B.2 A.HMG4C

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C***********************************************************************
C                                                                       -
C                       PREPARED 9/26/79 AT ANL                         -
C                                                                       -
CF          A.HMG4C                                                     -
CE          INPUT FOR CCCC TO ARC SYSTEM CROSS SECTION HOMOGENIZATION   -
C                                                                       -
CN                      THIS IS A USER-SUPPLIED BCD DATA SET.           -
CN                      THE LIST FOR EACH RECORD IS GIVEN IN TERMS      -
CN                      OF THE BCD FORMAT OF THAT DATA CARD.            -
CN                      COLUMNS 1-2 NORMALLY CONTAIN THE CARD TYPE      -
CN                      NUMBER.                                         -
CN                      A BLANK FIELD GIVES THE DEFAULT OPTION          -
CN                      INDICATED.                                      -
CN                      ALL INPUT CARDS ARE OPTIONAL.                   -
C                                                                       -
C***********************************************************************

C-----------------------------------------------------------------------
CR          PROBLEM TITLE (TYPE 01)                                     -
C                                                                       -
CL    FORMAT------(I2,4X,11A6)                                          -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      01                                                       -
CD                                                                      -
CD    7-72     ANY ALPHANUMERIC CHARACTERS.                             -
C                                                                       -
CN              UP TO SIX TYPE 01 CARDS MAY BE USED.                    -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          PROBLEM OPTIONS (TYPE 02)                                   -
C                                                                       -
CL    FORMAT------(I2,4X,8I6)                                           -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      02                                                       -
CD                                                                      -
CD    7-12     SIZE OF MAIN CORE CONTAINER ARRAY IN REAL*8 WORDS        -
CD             (SINGLE WORDS ON CDC SYSTEMS). (DEFAULT=20000).          -
CD                                                                      -
CD    13-18    PRINT FILE MASTER CONTROL FLAG.                          -
CD             0...PRINT GENERAL RUN INFORMATION AND REQUESTED EDITS    -
CD                 (DEFAULT).                                           -
CD             1...SUPPRESS ALL PRINTING EXCEPT DIAGNOSTICS.            -
CD                                                                      -
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CD    19-24     COMPXS EDIT FLAG.                                          -
CD              0...NO EDIT (DEFAULT).                                     -
CD              1...PRINT COMPLETE EDIT OF THE CREATED COMPXS FILE.        -
CD              2...WRITE COMPLETE EDIT OF THE CREATED COMPXS FILE         -
CD                  ON THE AUXILIARY OUTPUT FILE.                          -
CD              3...COMPXS EDIT WRITTEN ON BOTH PRINT AND AUXILIARY        -
CD                  OUTPUT FILES.                                          -
CD                                                                         -
CD    25-30     ISOTXS EDIT FLAG.                                          -
CD              0...NO EDIT (DEFAULT).                                     -
CD              1...PRINT RUNNING EDIT OF ISOTXS (I.E. NOT EVERY           -
CD                  ISOTOPE ON THE FILE IS PRINTED, ONLY THOSE             -
CD                  ACTUALLY REFERENCED).                                  -
CD              2...WRITE RUNNING EDIT OF ISOTXS ON THE AUXILIARY          -
CD                  OUTPUT FILE.                                           -
CD              3...RUNNING EDIT OF ISOTXS WRITTEN ON BOTH PRINT           -
CD                  AND AUXILIARY OUTPUT FILES.                            -
CD                                                                         -
CD    31-36     POINTR DEBUGGING EDIT FLAG.                                -
CD              0...NO DEBUGGING PRINTOUT (DEFAULT).                       -
CD              1...DUMP PRINTOUTS ONLY.                                   -
CD              2...TRACE PRINTOUTS ONLY.                                  -
CD              3...BOTH TRACE AND DUMP PRINTOUT.                          -
CD                                                                         -
CD              NOTE THAT HMG4C CONTAINS NO DUMPS, I.E. 1 IS NOT           -
CD              A RELEVANT VALUE FOR THIS FLAG.                            -
CD                                                                         -
CD    37-42     PROMPT FISSION SPECTRUM OPTION FLAG.                       -
CD              0...IGNORE ISOTOPE FISSION VECTORS, IF PRESENT IN          -
CD                  ISOTXS, AND USE THE SET FISSION VECTOR FOR ALL         -
CD                  COMPOSITIONS (DEFAULT). IF A SET FISSION SPECTRUM      -
CD                  IS NOT PRESENT IN ISOTXS, THE COMPOSITION FISSION      -
CD                  SPECTRA WILL BE COMPUTED BY THE TOTAL FISSION          -
CD                  SOURCE WEIGHTING METHOD USING ISOTOPE FISSION          -
CD                  VECTORS.                                               -
CD              1...USE ISOTOPE FISSION VECTORS, IF PRESENT IN ISOTXS,     -
CD                  TO COMPUTE COMPOSITION FISSION VECTORS WITH TOTAL      -
CD                  FISSION SOURCE WEIGHTING, I.E., UNDER ASSUMPTION       -
CD                  THAT FLUX IS GROUP INDEPENDENT. THIS IS THE            -
CD                  PREFERRED WEIGHTING METHOD. IF AN ISOTOPE FISSION      -
CD                  VECTOR IS NOT PRESENT, THE SET FISSION VECTOR WILL     -
CD                  BE USED IN ITS PLACE.                                  -
CD              2...USE ISOTOPE FISSION VECTORS, IF PRESENT IN ISOTXS,     -
CD                  TO COMPUTE COMPOSITION FISSION VECTORS WITH            -
CD                  NU*SIGMA(FISSION) WEIGHTING. THIS METHOD OF            -
CD                  COMPUTING A FISSION SPECTRUM IS NOT RECOMMENDED.       -
CD                  IF AN ISOTOPE FISSION VECTOR IS NOT PRESENT, THE       -
CD                  SET FISSION VECTOR WILL BE USED IN ITS PLACE.          -
CD                                                                         -
CD    43-48     AUXILIARY OUTPUT FILE MASTER CONTROL FLAG.                 -
CD              0...SUPPRESS ALL OUTPUT TO AUXILIARY FILE (DEFAULT).       -
CD              1...WRITE GENERAL RUN INFORMATION AND REQUESTED            -
CD                  EDITS ON AUXILIARY OUTPUT FILE.                        -
CD                                                                         -
CD              NOTE THAT ERROR DIAGNOSTICS ARE NOT WRITTEN ON THE         -
CD              AUXILIARY OUTPUT FILE.                                     -
CD                                                                         -
CD    49-54     EDIT FLAG FOR A SUPPLIED COMPXS FILE.                      -
CD              0...NO EDIT (DEFAULT).                                     -
CD              1...PRINT COMPLETE EDIT OF SUPPLIED COMPXS FILE.           -
CD              2...WRITE COMPLETE EDIT OF SUPPLIED COMPXS FILE ON         -
CD                  THE AUXILIARY OUTPUT FILE.                             -
CD              3...EDIT OF SUPPLIED COMPXS WRITTEN ON BOTH PRINT AND      -
CD                  AUXILIARY OUTPUT FILES.                                -
C                                                                          -
C----------------------------------------------------------------------------

C----------------------------------------------------------------------------
C                                                                          -
CR          SCATTERING CROSS SECTION TRUNCATION OPTION  (TYPE 03)          -
C                                                                          -
CL    FORMAT-----(I2,4X,E12.5)                                             -
C                                                                          -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                     -
CD    -------  ------------------------------------------------------------
CD    1-2      03                                                          -
CD                                                                         -
CD    7-18     SCATTERING MATRIX TRUNCATION FRACTION (DEFAULT=1.0)         -
C                                                                          -
CN              THE SCATTERING CROSS SECTION BANDWIDTH OF A                -
CN              COMPOSITION IN FILE COMPXS IS TRUNCATED AT                 -
CN              THE POINT WHERE THE INPUT FRACTION (COL 7-18)              -
CN              OF THE TOTAL SCATTERING CROSS SECTION HAS                  -
CN              BEEN ACCUMULATED.  A VALUE OF .999 IS                      -
CN              GENERALLY SUFFICIENT TO RETAIN THE RIGOR                   -
CN              OF A CALCULATION WHILE SIGNIFICANTLY REDUCING              -
CN              THE SCATTERING BANDWIDTH AND HENCE, THE I/O                -
CN              TIMES ASSOCIATED WITH THE SCATTERING SOURCE                -
CN              DETERMINATION IN A NEUTRONICS CALCULATION.                 -
C                                                                          -
C----------------------------------------------------------------------------

CEOF
```

B.3 A.ISO (SEE ISOTXS FILE DESCRIPTION)

B.4 A.NIP3

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C*****************************************************************************
C                                                                             -
C                     PREPARED 8/28/75 AT ANL                                 -
C                     LAST REVISED 09/30/83                                   -
C                                                                             -
CF          A.NIP3                                                            -
CE          NEUTRONICS MODEL INPUT FOR CODES WHICH REQUIRE CCCC                -
CE          INTERFACE FILES                                                   -
C                                                                             -
CN                    THIS BCD DATA SET MAY BE WRITTEN EITHER                 -
CN                    IN FREE FORMAT (UNFORM=A.NIP3) OR ACCORDING TO          -
CN                    THE FORMATS SPECIFIED FOR EACH CARD TYPE                -
CN                    (DATASET=A.NIP3).                                       -
CN                                                                            -
CN                    COLUMNS 1-2 MUST CONTAIN THE CARD TYPE                  -
CN                    NUMBER.                                                 -
CN                                                                            -
CN                    UNLESS OTHERWISE STATED, BLANKS ARE NOT                 -
CN                    MEANINGFUL IN A6 LABEL FIELDS.                          -
C                                                                             -
C                                                                             -
CN                 *** CARD TYPE DIRECTORY ***                                -
CN                                                                            -
CN    TYPE                      CONTENTS                                      -
CN    ====    ================================================              -
CN     01     PROBLEM TITLE                                                  -
CN     02     INPUT PROCESSING SPECIFICATIONS                                -
CN     03     PROBLEM GEOMETRY                                               -
CN     04     EXTERNAL BOUNDARY CONDITIONS                                   -
CN     05     EXTERNAL BOUNDARY CONDITION CONSTANTS                          -
CN     06     REGION BOUNDARIES FOR ORTHOGONAL GEOMETRIES                    -
CN     07     AREA SPECIFICATIONS                                            -
CN     09     VARIABLE-MESH STRUCTURE                                        -
CN     10     INTERNAL BLACK ABSORBER CONDITIONS                             -
CN     11     INTERNAL BLACK ABSORBER CONDITION CONSTANTS                    -
CN     12     FINITE-GEOMETRY TRANSVERSE DISTANCES                           -
CN     13     MATERIAL SPECIFICATIONS                                        -
CN     14     COMPOSITION (ZONE) SPECIFICATIONS                              -
CN     15     REGION/COMPOSITION CORRESPONDENCE                              -
CN     19     REGION OR MESH DISTRIBUTED INHOMOGENEOUS SOURCE                -
CN     21     SEARCH EDIT OPTIONS AND CONVERGENCE CRITERIA                   -
CN     22     SEARCH PARAMETER DATA                                          -
CN     23     CONCENTRATION MODIFIERS FOR CRITICALITY SEARCH                 -
CN     24     MESH MODIFIERS FOR CRITICALITY SEARCH                          -
CN     25     BUCKLING MODIFIERS FOR CRITICALITY SEARCH                      -
CN     26     ALPHA MODIFIERS FOR CRITICALITY SEARCH                         -
CN     29     HEXAGON DIMENSION                                              -
CN     30     REGION DEFINITIONS FOR ARRAYS OF HEXAGONS                      -
CN     31     BACKGROUND REGION FOR ARRAYS OF HEXAGONS                       -
CN     34     COMPOSITION- AND GROUP-DEPENDENT BUCKLINGS                     -
CN     35     DIRECTIONAL DIFFUSION COEF. SCHEME                             -
CN     36     DIRECTIONAL DIFFUSION COEF./COMPOSITION CORRESPONDENCE         -
CN     37     FISSION ENERGY CONVERSION FACTORS                              -
CN     38     CAPTURE ENERGY CONVERSION FACTORS                              -
CN     39     NUCLIDE SET ASSIGNMENTS                                        -
CN     40     SOURCE EDIT, SYNTHESIS TRIAL FUNCTION SOURCE                   -
CN     41     NATURAL DECAY INHOMOGENEOUS SOURCE                             -
CN     42     SOURCE SPECTRA                                                 -
CN     43     GRAPHICS OUTPUT CONTROL                                        -
CN     44     ASSIGNMENT OF REGION TO CONTROL ROD BANK                       -
C                                                                             -
C*****************************************************************************


C-----------------------------------------------------------------------------
CR          PROBLEM TITLE (TYPE 01)                                           -
C                                                                             -
CL    FORMAT------(I2,4X,11A6)                                                -
C                                                                             -
CD    COLUMNS           CONTENTS...IMPLICATIONS, IF ANY                       -
CD    =======   =================================================           -
CD    1-2       01                                                            -
CD                                                                            -
CD    7-72      ANY ALPHANUMERIC CHARACTERS.                                  -
C                                                                             -
CN                ANY NUMBER OF TYPE 01 CARDS MAY BE USED.                    -
C                                                                             -
C-----------------------------------------------------------------------------


C-----------------------------------------------------------------------------
CR          INPUT PROCESSING SPECIFICATION (TYPE 02)                          -
C                                                                             -
CL    FORMAT------(I2,10X,8I6)                                                -
C                                                                             -
CD    COLUMNS           CONTENTS...IMPLICATIONS, IF ANY                       -
CD    =======   =================================================           -
CD    1-2       02                                                            -
CD                                                                            -
CD    13-18     POINTR DEBUGGING EDIT FOR GEOMETRY PROCESSING MODULE.         -
CD              0...NO DEBUGGING PRINTOUT (DEFAULT).                          -
CD              1...DEBUGGING DUMP PRINTOUT.                                  -
CD              2...DEBUGGING TRACE PRINTOUT.                                 -
CD              3...FULL DEBUGGING PRINTOUT (DUMP+TRACE).                     -
CD                                                                            -
CD    19-24     GEOMETRY PROCESSING MODULE EDIT.                              -
CD              0...NO EDITS (DEFAULT).                                       -
CD              1...PRINT GEOMETRY EDITS.                                     -
CD              2...WRITE GEOMETRY EDITS TO AUXILIARY OUTPUT FILE.            -
CD              3...GEOMETRY EDITS GO TO BOTH PRINT AND AUXILIARY             -
CD                  OUTPUT FILES.                                             -
CD                                                                            -
CD              OPTIONS 2 AND 3 ARE OPERATIVE ONLY FOR THOSE CODES            -
CD              WHICH RECOGNIZE AUXILIARY OUTPUT FILES.                       -
CD                                                                            -
CD    25-30     SIZE OF MAIN CORE STORAGE ARRAY FOR GEOMETRY                  -
```

```
CD              PROCESSING MODULE (GNIP4C) IN REAL*8 WORDS
CD              (DEFAULT=10000).
CD
CD    31-36     SIZE OF BULK CORE STORAGE ARRAY FOR GEOMETRY
CD              PROCESSING MODULE (GNIP4C) IN REAL*8 WORDS
CD              (DEFAULT=0).
CD
CD    37-42     SIZE OF MAIN CORE STORAGE ARRAY FOR CROSS SECTION
CD              PROCESSING MODULES IN REAL*8 WORDS (DEFAULT = 20000).
CD
CD    43-48     SIZE OF BULK CORE STORAGE ARRAY FOR CROSS SECTION
CD              PROCESSING MODULES IN REAL*8 WORDS (DEFAULT=0).
CD
CD    49-54     POINTR DEBUGGING EDIT FOR CROSS SECTION PROCESSING
CD              MODULES.
CD              0...NO DEBUGGING PRINTOUT (DEFAULT).
CD              1...DEBUGGING DUMP PRINTOUT.
CD              2...DEBUGGING TRACE PRINTOUT.
CD              3...FULL DEBUGGING PRINTOUT (DUMP+TRACE).
CD
CD    55-60     CROSS SECTION PROCESSING EDIT.
CD              0...NO EDITS (DEFAULT).
CD              1...PRINT CROSS SECTION EDITS.
CD              2...WRITE CROSS SECTION EDITS TO AUXILIARY OUTPUT FILE.
CD              3...CROSS SECTION EDITS GO TO BOTH PRINT AND AUXILIARY
CD                  OUTPUT FILES.
CD
CD    61-66     REGION/MESH INTERVAL PRINTER-PLOTTER MAP EDIT DURING
CD              GEOMETRY PROCESSING.
CD              0...NO MAP (DEFAULT).
CD              1...PRINT REGION MAP.
CD              2...WRITE REGION MAP TO AUXILIARY OUTPUT FILE.
CD              3...WRITE REGION MAP TO BOTH PRINT AND AUXILIARY OUTPUT
CD                  FILES.
CD
CD    67-72     ZONE(COMPOSITION)/MESH INTERVAL PRINTER-PLOTTER MAP
CD              EDIT DURING GEOMETRY PROCESSING.
CD              0...NO MAP (DEFAULT).
CD              1...PRINT ZONE MAP.
CD              2...WRITE ZONE MAP TO AUXILIARY OUTPUT FILE.
CD              3...WRITE ZONE MAP TO BOTH PRINT AND AUXILIARY OUTPUT
CD                  FILES.
CD
CN              EDIT OPTIONS 2 AND 3 ARE OPERATIVE ONLY FOR THOSE
CN              CODES WHICH RECOGNIZE AUXILIARY OUTPUT FILES.
CN
CN              THE PRINTER-PLOTTER MAP OPTIONS (COLS. 61-72) ARE
CN              ENTIRELY SEPARATE FROM THE GRAPHICS MAP OPTIONS
CN              IN COLS. 7-48 OF THE TYPE 43 CARD.
C
C---------------------------------------------------------------------
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C---------------------------------------------------------------------
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CR          PROBLEM GEOMETRY SPECIFICATION (TYPE 03)
C
CL    FORMAT-----(I2,10X,I6)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY.
CD    =======   ==========================================================
CD    1-2       03
CD
CD    13-18     GEOMETRY TYPE.
CD              10...SLAB
CD              20...CYLINDER
CD              30...SPHERE
CD              40...X-Y
CD              44...X-Y-Z
CD              50...R-Z
CD              60...R-THETA
CD              62...R-THETA-Z
CD              64...THETA-R
CD              66...THETA-R-Z
CD              70...TRIANGULAR, RHOMBIC BOUNDARY, CORE CENTER AT
CD                   60 DEGREE ANGLE (SIXTH CORE SYMMETRY).
CD              72...TRIANGULAR, RECTANGULAR BOUNDARY, HALF CORE
CD                   SYMMETRY.
CD              74...TRIANGULAR, RHOMBIC BOUNDARY, CORE CENTER AT
CD                   120 DEGREE ANGLE (THIRD CORE SYMMETRY).
CD              76...TRIANGULAR, 60 DEGREE TRIANGULAR BOUNDARY,
CD                   SIXTH CORE SYMMETRY.
CD              78...TRIANGULAR, RECTANGULAR BOUNDARY, QUARTER
CD                   CORE SYMMETRY.
CD              80...TRIANGULAR, RECTANGULAR BOUNDARY, FULL CORE.
CD              90...TRIANGULAR-Z, RHOMBIC BOUNDARY IN PLANE, CORE
CD                   CENTER LINE AT 60 DEGREE ANGLE.
CD              92...TRIANGULAR-Z, RECTANGULAR BOUNDARY IN PLANE,
CD                   HALF CORE SYMMETRY IN PLANE.
CD              94...TRIANGULAR-Z, RHOMBIC BOUNDARY IN PLANE, CORE
CD                   CENTER LINE AT 120 DEGREE ANGLE.
CD              96...TRIANGULAR-Z, 60 DEGREE TRIANGULAR BOUNDARY
CD                   IN PLANE.
CD              98...TRIANGULAR-Z, RECTANGULAR BOUNDARY IN PLANE,
CD                   QUARTER CORE SYMMETRY IN PLANE.
CD             100...TRIANGULAR-Z, RECTANGULAR BOUNDARY IN PLANE,
CD                   FULL CORE IN PLANE.
CD             110...HEXAGONAL, FULL CORE.
CD             114...HEXAGONAL, SIXTH CORE SYMMETRY.
CD             116...HEXAGONAL, THIRD CORE SYMMETRY.
CD             120...HEXAGONAL-Z, FULL CORE IN PLANE.
CD             124...HEXAGONAL-Z, SIXTH CORE SYMMETRY IN PLANE.
CD             126...HEXAGONAL-Z, THIRD CORE SYMMETRY IN PLANE.
CD
C
C
C---------------------------------------------------------------------
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C-------------------------------------------------------------------
CR          EXTERNAL BOUNDARY CONDITIONS (TYPE 04)                  -
C                                                                   -
CL     FORMAT-----(I2,10X,616)                                      -
C                                                                   -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY             -
CD     =======  ==========================================         -
CD     1-2      04                                                  -
CD                                                                  -
CD     13-18    BOUNDARY CONDITION AT LOWER "X" BOUNDARY OF REACTOR. -
CD                                                                  -
CD     19-24    BOUNDARY CONDITION AT UPPER "X" BOUNDARY OF REACTOR. -
CD                                                                  -
CD     25-30    BOUNDARY CONDITION AT LOWER "Y" BOUNDARY OF REACTOR. -
CD                                                                  -
CD     31-36    BOUNDARY CONDITION AT UPPER "Y" BOUNDARY OF REACTOR. -
CD                                                                  -
CD     37-42    BOUNDARY CONDITION AT LOWER Z BOUNDARY OF REACTOR.   -
CD                                                                  -
CD     43-48    BOUNDARY CONDITION AT UPPER Z BOUNDARY OF REACTOR.   -
CD                                                                  -
CD                                                                  -
CD              2...PHI=0.                                          -
CD              3...PHI PRIME=0.                                    -
CD              4...D * PHI PRIME + A * PHI = 0.                    -
CD              6...REPEATING (PERIODIC) WITH OPPOSITE FACE.        -
CD              7...REPEATING (PERIODIC) WITH NEXT ADJACENT BOUNDARY -
CD                  (SEE DISCUSSION BELOW).                         -
CD              8...INVERTED REPEATING ALONG THIS FACE              -
CD                  (180 DEGREE ROTATION).                          -
CD              9...INCOMING ANGULAR FLUX ZERO (TRANSPORT ONLY).    -
CD              10..REFLECTIVE (TRANSPORT ONLY).                    -
CD              11..PERIODIC (TRANSPORT ONLY).                      -
CD              12..WHITE (TRANSPORT ONLY).                         -
CD                                                                  -
C                                                                   -
CN              PHI PRIME IS THE DERIVATIVE OF THE FLUX IN THE      -
CN              DIRECTION OF THE REACTOR OUTWARD NORMAL. D IS THE   -
CN              DIFFUSION COEFFICIENT IN THE MESH INTERVAL          -
CN              IMMEDIATELY INSIDE THE REACTOR BOUNDARY. IF COLS.   -
CN              43-48 ARE 4 AND NO TYPE 05 CARD IS SUPPLIED TO SPECIFY -
CN              THE CONSTANT A, THE VALUE 0.46920 WILL BE USED BY   -
CN              DEFAULT.                                            -
CN                                                                  -
CN              CONDITIONS 2-8 APPLY TO DIFFUSION THEORY PROBLEMS,  -
CN              AND 9-12 APPLY TO TRANSPORT THEORY PROBLEMS.        -
CN                                                                  -
CN              "X" REPRESENTS THE FIRST DIMENSION COORDINATE (X IN -
CN              X-Y GEOMETRY, R IN R-Z, ETC.). "Y" REPRESENTS THE   -
CN              SECOND DIMENSION COORDINATE (Y IN X-Y GEOMETRY, Z IN -
CN              R-Z, ETC.). WHEN THE MODEL IS THREE-DIMENSIONAL, THE -
CN              THIRD DIMENSION IS ALWAYS Z.                        -
CN                                                                  -
CN              REPEATING CONDITIONS (6,7,8) ARE ONLY APPLICABLE TO -
CN              THE FIRST TWO DIMENSIONS.                           -
CN                                                                  -
CN              NOTE FOR REPEATING CONDITION 7.  LET XL DENOTE THE  -
CN              LOWER "X" BOUNDARY, XU DENOTE THE UPPER "X" BOUNDARY, -
CN              YL DENOTE THE LOWER "Y" BOUNDARY AND YU DENOTE THE  -
CN              UPPER Y BOUNDARY.  FOR REPEATING BOUNDARY CONDITIONS -
CN              (CONDITION 7), THE SEQUENCE OF BOUNDARIES IMPLIED BY -
CN              THE TERM "NEXT ADJACENT BOUNDARY" IS XL, YL, XU, YU. -
CN              OF THE TWO BOUNDARIES INVOLVED, THE ONE APPEARING   -
CN              FIRST IN THE SEQUENCE IS ASSIGNED THE BOUNDARY      -
CN              CONDITION (7), THE SECOND IS IGNORED.  FOR EXAMPLE, -
CN              IF XL AND YL ARE THE PERIODIC BOUNDARIES, COLS. 13-18 -
CN              MUST CONTAIN A 7, COLS. 25-30 WILL BE IGNORED.      -
C                                                                   -
C-------------------------------------------------------------------
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C-------------------------------------------------------------------
CR          EXTERNAL BOUNDARY CONDITION CONSTANTS (TYPE 05)         -
C                                                                   -
CL     FORMAT-----(I2,8X,A2,E12.5,12X,2I6)                          -
C                                                                   -
CD     COLUMNS     CONTENTS...IMPLICATIONS, IF ANY                 -
CD     =======  ==========================================         -
CD     1-2      05                                                  -
CD                                                                  -
CD     11-12    BOUNDARY DESIGNATOR.                                -
CD              XL..."X" LOWER.                                     -
CD              XU..."X" UPPER.                                     -
CD              YL..."Y" LOWER.                                     -
CD              YU..."Y" UPPER.                                     -
CD              ZL...Z LOWER.                                       -
CD              ZU...Z UPPER.                                       -
CD                                                                  -
CD     13-24    VALUE OF CONSTANT A REFERRED TO ON CARD TYPE 04.    -
CD                                                                  -
CD     37-42    HIGHER-ENERGY GROUP NUMBER FOR WHICH CONSTANTS APPLY. -
CD                                                                  -
CD     43-48    LOWER-ENERGY GROUP NUMBER FOR WHICH CONSTANTS APPLY. -
C                                                                   -
CN              AS MANY TYPE 05 CARDS AS NECESSARY MAY BE USED TO   -
CN              SPECIFY THE EXTERNAL BOUNDARY CONDITIONS.           -
CN                                                                  -
CN              IF NO "HIGHER-ENERGY GROUP NUMBER" IS SUPPLIED (COLS. -
CN              37-42 ARE BLANK), THE CONSTANTS GIVEN APPLY TO ALL  -
CN              ENERGY GROUPS. IF NO "LOWER-ENERGY GROUP NUMBER" IS -
CN              SUPPLIED (COLS. 43-48 ARE BLANK), THE CONSTANTS GIVEN -
CN              APPLY TO THE "HIGHER-ENERGY GROUP" ONLY. IF NO GROUP -
CN              NUMBERS ARE SUPPLIED (COLS. 37-48 ARE BLANK), THE   -
CN              CONSTANTS GIVEN APPLY TO ALL ENERGY GROUPS.         -
CN                                                                  -
CN              DATA ON THIS CARD MAY BE OVERLAYED. THAT IS, BOUNDARY -
CN              CONSTANTS DEFINED ON LATER TYPE 5 CARDS SUPERCEDE DATA -
CN              FOR ENERGY RANGES PREVIOUSLY SPECIFIED.             -
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CN                                                                    -
CN            "X" REPRESENTS THE FIRST DIMENSION COORDINATE (X IN     -
CN            SECOND DIMENSION COORDINATE (Y IN X-Y GEOMETRY, Z IN    -
CN            X-Y GEOMETRY, R IN R-Z, ETC.). "Y" REPRESENTS THE       -
CN            R-Z, ETC.). WHEN THE MODEL IS THREE-DIMENSIONAL, THE    -
CN            THIRD DIMENSION IS ALWAYS Z.                            -
C                                                                     -
C---------------------------------------------------------------------
C---------------------------------------------------------------------
CR          REGION BOUNDARY COORDINATES AND CONSTANT MESH STRUCTURE    -
CR          (TYPE 06)                                                 -
C                                                                     -
CL    FORMAT-----(I2,4X,A6,2E12.5,2I6,2E12.5)                         -
C                                                                     -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD    =======  ========================================================
CD    1-2      06                                                     -
CD                                                                    -
CD    7-12     REGION LABEL (REPEATED ON ADDITIONAL TYPE 06 CARDS).   -
CD                                                                    -
CD    13-24    "X"-DIRECTION LOWER-BOUNDARY COORDINATE.               -
CD                                                                    -
CD    25-36    "X"-DIRECTION UPPER-BOUNDARY COORDINATE.               -
CD                                                                    -
CD    37-42    FOR ONE-DIMENSIONAL AND TWO-DIMENSIONAL GEOMETRIES,    -
CD             NUMBER OF INTERVALS IN "X"-DIRECTION.                  -
CD                                                                    -
CD                                  ** OR **                          -
CD                                                                    -
CD             FOR THREE-DIMENSIONAL GEOMETRIES, LOWER Z MESH         -
CD             LINE NUMBER OF THE REGION.                             -
CD                                                                    -
CD    43-48    FOR TWO-DIMENSIONAL GEOMETRIES, NUMBER OF INTERVALS    -
CD             IN "Y"-DIRECTION.                                      -
CD                                                                    -
CD                                  ** OR **                          -
CD                                                                    -
CD             FOR THREE-DIMENSIONAL GEOMETRIES, UPPER Z MESH         -
CD             LINE NUMBER OF THE REGION.                             -
CD                                                                    -
CD    49-60    "Y"-DIRECTION LOWER-BOUNDARY COORDINATE.               -
CD                                                                    -
CD    61-72    "Y"-DIRECTION UPPER-BOUNDARY COORDINATE.               -
C                                                                     -
CN            CARD TYPE 06 IS NOT PERTINENT FOR TRIANGULAR,           -
CN            TRIANGULAR-Z, HEXAGONAL, OR HEXAGONAL-Z GEOMETRIES.     -
CN            SEE CARD TYPE 30.                                       -
CN                                                                    -
CN            "X" REPRESENTS THE FIRST DIMENSION COORDINATE (X IN     -
CN            X-Y GEOMETRY, R IN R-Z, ETC.). "Y" REPRESENTS THE       -
CN            SECOND DIMENSION COORDINATE (Y IN X-Y GEOMETRY, Z IN    -
CN            R-Z, ETC.). WHEN THE MODEL IS THREE-DIMENSIONAL, THE    -
CN            THIRD DIMENSION IS ALWAYS Z.                            -
C                                                                     -
CN            IN GEOMETRIES INVOLVING AN ANGULAR DIMENSION (THETA)    -
CN            THE ANGULAR VARIABLE MUST BE GIVEN IN RADIANS.          -
CN                                                                    -
CN            REGIONS MAY BE DEFINED USING THE OVERLAY PRECEDURE,     -
CN            WITH THE LATEST REGION ASSIGNMENT OVERLAYING THE        -
CN            PREVIOUS CONFIGURATION, OR USING THE USUAL PROCEDURE,   -
CN            WITH EACH REGION'S BOUNDARIES GIVEN EXPLICITLY.         -
CN            REGION LABELS MUST BE NON-BLANK.                        -
CN                                                                    -
CN            THE MESH FOR A DIRECTION MUST BE COMPLETELY SPECIFIED   -
CN            EITHER ON THE TYPE 06 OR 09 CARDS. IF MESH DATA ARE     -
CN            SUPPLIED ON BOTH TYPE 06 AND 09 CARDS, THE TYPE 09      -
CN            DATA WILL BE USED.                                      -
CN                                                                    -
CN            FOR ONE-DIMENSIONAL PROBLEMS, ONLY THE "X"-DIRECTION    -
CN            UPPER BOUNDARIES NEED BE GIVEN FOR REGIONS AFTER THE    -
CN            FIRST.  IF THIS OPTION IS USED THE TYPE 6 CARDS MUST    -
CN            BE ARRANGED SO AS TO DEFINE REGIONS SEQUENTIALLY,       -
CN            MOVING FROM LEFT TO RIGHT.  IN OTHER WORDS THE          -
CN            X-DIRECTION UPPER BOUNDARIES MUST BE IN ASCENDING       -
CN            ORDER.                                                  -
CN                                                                    -
CN            FOR THREE-DIMENSIONAL GEOMETRIES, THE DEFINITION OF     -
CN            THE MESH STRUCTURE MUST BE SUPPLIED ON TYPE 09 CARDS.   -
CN                                                                    -
CN            THE LOWEST Z MESH LINE NUMBER (CORRESPONDING TO THE     -
CN            FIRST Z BOUNDARY) OF THE MODEL IS 0 (ZERO). THE         -
CN            LARGEST Z MESH LINE NUMBER (CORRESPONDING TO THE        -
CN            SECOND Z BOUNDARY) IS EQUAL TO THE NUMBER OF Z MESH     -
CN            INTERVALS.                                              -
C                                                                     -
C---------------------------------------------------------------------
C---------------------------------------------------------------------
CR              AREA SPECIFICATIONS (TYPE 07)                         -
C                                                                     -
CL    FORMAT-----(I2,4X,11A6)                                         -
C                                                                     -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD    =======  ========================================================
CD    1-2      07                                                     -
CD                                                                    -
CD    7-12     AREA LABEL (REPEATED ON ADDITIONAL TYPE 07 CARDS).     -
CD                                                                    -
CD    13-18    LABEL OF REGION COMPRISING AREA.                       -
CD                                                                    -
CD    19-24    LABEL OF REGION COMPRISING AREA.                       -
CD                                                                    -
CD    25-30    LABEL OF REGION COMPRISING AREA.                       -
CD                                                                    -
CD    31-36    LABEL OF REGION COMPRISING AREA.                       -
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CD                                                                      -
CD     37-42      LABEL OF REGION COMPRISING AREA.                      -
CD                                                                      -
CD     43-48      LABEL OF REGION COMPRISING AREA.                      -
CD                                                                      -
CD     49-54      LABEL OF REGION COMPRISING AREA.                      -
CD                                                                      -
CD     55-60      LABEL OF REGION COMPRISING AREA.                      -
CD                                                                      -
CD     61-66      LABEL OF REGION COMPRISING AREA.                      -
CD                                                                      -
CD     67-72      LABEL OF REGION COMPRISING AREA.                      -
C                                                                       -
CN                AREA LABELS MUST BE NON-BLANK. THE FIRST BLANK REGION -
CN                LABEL ENCOUNTERED TERMINATES READING OF THE DATA ON   -
CN                THAT PARTICULAR TYPE 07 CARD. A REGION CAN BE PLACED  -
CN                IN AS MANY AREAS AS THE USER DESIRES.                 -
CN                                                                      -
CN                THE CONCEPT OF AREAS DOES NOT EXIST IN THE CCCC       -
CN                ENVIRONMENT. ONLY CERTAIN CODES WRITTEN AT ANL MAKE   -
CN                USE OF AREAS, AND IN THOSE CODES AREAS ARE USED FOR   -
CN                EDIT PURPOSES ONLY.                                   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR            VARIABLE-MESH STRUCTURE (TYPE 09)                         -
C                                                                       -
CL     FORMAT-----(I2,9X,A1,3(I6,E12.5))                                -
C                                                                       -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                 -
CD     =======  ==============================================         -
CD     1-2      09                                                      -
CD                                                                      -
CD     12       COORDINATE DIRECTION.                                   -
CD              X..."X" COORDINATE DIRECTION.                           -
CD              Y..."Y" COORDINATE DIRECTION.                           -
CD              Z...Z-COORDINATE DIRECTION.                             -
CD                                                                      -
CD     13-18    NUMBER OF INTERVALS.                                    -
CD                                                                      -
CD     19-30    UPPER COORDINATE.                                       -
CD                                                                      -
CD     31-36    NUMBER OF INTERVALS.                                    -
CD                                                                      -
CD     37-48    UPPER COORDINATE.                                       -
CD                                                                      -
CD     49-54    NUMBER OF INTERVALS.                                    -
CD                                                                      -
CD     55-66    UPPER COORDINATE.                                       -
C                                                                       -
CN              NOTE THAT A Z IN COL. 12 IS PERTINENT ONLY IF THE       -
CN              GEOMETRY IS THREE-DIMENSIONAL.                          -
CN                                                                      -
CN              "X" REPRESENTS THE FIRST DIMENSION COORDINATE (X IN     -
CN              X-Y GEOMETRY, R IN R-Z, ETC.). "Y" REPRESENTS THE       -
CN              SECOND DIMENSION COORDINATE (Y IN X-Y GEOMETRY, Z IN    -
CN              R-Z, ETC.). WHEN THE MODEL IS THREE-DIMENSIONAL, THE    -
CN              THIRD DIMENSION IS ALWAYS Z.                            -
C                                                                       -
CN              IN GEOMETRIES INVOLVING AN ANGULAR DIMENSION (THETA)    -
CN              THE ANGULAR VARIABLE MUST BE GIVEN IN RADIANS.          -
CN                                                                      -
CN              EACH NUMBER PAIR IS OF THE FORM (N(I), X(I)). THERE     -
CN              ARE N(I) INTERVALS BETWEEN X(I-1) AND X(I), WHERE X(0)  -
CN              IS THE LOWER REACTOR BOUNDARY IN THIS DIRECTION.        -
CN              NUMBER PAIRS MUST BE GIVEN IN ORDER OF INCREASING       -
CN              MESH COORDINATES. ALL REGION BOUNDARIES MUST COINCIDE   -
CN              WITH THE MESH LINES THAT BOUND MESH INTERVALS.          -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR            INTERNAL BLACK ABSORBER CONDITIONS (TYPE 10)               -
C                                                                       -
CL     FORMAT-----(I2,10X,10A6)                                         -
C                                                                       -
CD     COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                 -
CD     =======  ==============================================         -
CD     1-2      10                                                      -
CD                                                                      -
CD     13-18    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     19-24    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     25-30    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     31-36    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     37-42    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     43-48    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     49-54    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     55-60    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.         -
CD                                                                      -
CD     61-66    LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE         -
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CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.
CD
CD    67-72     LABEL OF COMPOSITION (CCCC ZONE) WHICH IS TO BE
CD              TREATED WITH INTERNAL BLACK BOUNDARY CONDITION.
C
CN              AS MANY TYPE 10 CARDS CAN BE USED AS ARE NECESSARY TO
CN              SPECIFY ALL OF THE DESIRED COMPOSITION (CCCC ZONE)
CN              LABELS.
CN
CN              EACH REGION WHICH IS COMPOSED OF ANY COMPOSITION
CN              LISTED ON TYPE 10 CARDS WILL BE TREATED AS A BLACK
CN              ABSORBER ACCORDING TO THE INTERNAL BOUNDARY CONDITIONS
CN              GIVEN ON TYPE 11 CARDS TO FOLLOW.
CN
CN              THE REGIONS WHICH ARE COMPRISED OF THESE COMPOSITIONS
CN              ARE SPECIFIED ON TYPE 15 CARDS.
CN
CN              THE FIRST BLANK COMPOSITION LABEL TERMINATES READING
CN              OF THE DATA ON THAT PARTICULAR TYPE 10 CARD.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          INTERNAL BLACK ABSORBER CONDITION CONSTANTS
CR          (TYPE 11)
C
CL    FORMAT-----(I2,10X,2E12.5,24X,216)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==========================================================
CD    1-2       11
CD
CD    13-24     THE CONSTANT A, DEFINED BELOW.
CD
CD    25-36     THE CONSTANT B, DEFINED BELOW.
CD
CD    61-66     HIGHER-ENERGY GROUP NUMBER FOR WHICH CONSTANTS APPLY.
CD
CD    67-72     LOWER-ENERGY GROUP NUMBER FOR WHICH CONSTANTS APPLY.
C
CN              THE INTERNAL BLACK BOUNDARY CONDITION IS SPECIFIED AS
CN
CN                        A*PHI PRIME + B/D*PHI = 0.
CN
CN              IF NO "HIGHER-ENERGY GROUP NUMBER" IS SUPPLIED (COLS.
CN              61-66 ARE BLANK), THE CONSTANTS GIVEN APPLY TO ALL
CN              ENERGY GROUPS. IF NO "LOWER-ENERGY GROUP NUMBER" IS
CN              SUPPLIED (COLS. 67-72 ARE BLANK), THE CONSTANTS GIVEN
CN              APPLY TO THE "HIGHER-ENERGY GROUP" ONLY. IF NO GROUP
CN              NUMBERS ARE SUPPLIED (COLS. 61-72 ARE BLANK), THE
CN              CONSTANTS GIVEN APPLY TO ALL ENERGY GROUPS.
CN
CN              DATA ON THIS CARD MAY BE OVERLAYED. THAT IS, CONSTANTS
CN              DEFINED ON LATER TYPE 11 CARDS SUPERCEDE DATA FOR
CN              ENERGY RANGES PREVIOUSLY SPECIFIED.
CN
CN              ANY GROUP FOR WHICH NO INTERNAL BLACK ABSORBER
CN              CONDITION CONSTANTS ARE SPECIFIED ON TYPE 11 CARDS
CN              WILL BE TREATED AS BEING NON-BLACK.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          FINITE-GEOMETRY TRANVERSE DISTANCES (TYPE 12)
C
CL    FORMAT-----(I2,4X,A6,4E12.5)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==========================================================
CD    1-2       12
CD
CD    7-12      REGION OR AREA LABEL.
CD
CD    13-24     ACTUAL TRANSVERSE HALF-HEIGHT OR RADIUS.
CD
CD    25-36     TRANSVERSE EXTRAPOLATION DISTANCE.
CD
CD    37-48     ACTUAL TRANSVERSE HALF-HEIGHT IN THE SECOND DIRECTION
CD              FOR A FINITE ONE-DIMENSIONAL RECTANGULAR SLAB.
CD
CD    49-60     TRANSVERSE EXTRAPOLATION DISTANCE IN THE SECOND
CD              DIRECTION FOR A FINITE ONE-DIMENSIONAL RECTANGULAR
CD              SLAB.
C
CN              THE DATA ON THE TYPE 12 CARDS ARE USED TO CALCULATE
CN              REGION VOLUMES AND, IN THE ABSENCE OF TYPE 34 CARDS,
CN              BUCKLINGS.  REGION VOLUMES ARE CALCULATED USING
CN              ACTUAL HALF-HEIGHTS (EXCLUDING THE EXTRAPOLATION
CN              DISTANCE).
CN
CN              AN AREA LABEL IN COLS. 7-12 IMPLIES ALL THE REGIONS
CN              ASSIGNED TO THAT AREA.
CN
CN              THE REGION-DEPENDENT DATA THAT IS PROVIDED ON THIS
CN              CARD IS CONVERTED BY THE GNIP4C INPUT PROCESSOR TO
CN              COMPOSITION-DEPENDENT DATA.  THIS IS A POTENTIAL
CN              PROBLEM FOR USERS IF THEY HAVE ASSIGNED ONE
CN              COMPOSITION TO TWO OR MORE REGIONS WITH DIFFERENT
CN              HALF HEIGHTS.
CN
CN              IF THERE IS NO REGION LABEL (COLS.7-12 ARE BLANK), THE
CN              DATA ON THE CARD APPLY TO ALL REGIONS OF THE REACTOR.
CN              IF THERE IS NO REGION LABEL AND IF THERE ARE NO TYPE 34-
CN              CARD (COMPOSITION AND GROUP DEPENDENT BUCKLING
CN              SPECIFICATIONS), THE DATA ON THIS CARD WILL BE USED TO
CN              CALCULATE A SPACE- AND ENERGY-INDEPENDENT BUCKLING AND
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CN              TO CALCULATE REGION VOLUMES. IN THIS MODE OF INPUT      -
CN              ONLY ONE TYPE 12 CARD SHOULD BE SUPPLIED.               -
CN                                                                      -
CN              IF MORE THAN ONE TYPE 12 CARD IS PRESENT (EACH CARD     -
CN              WITH A VALID REGION OR AREA LABEL IN COLS. 7-12), THE   -
CN              DATA ON THE CARDS WILL BE USED TO CALCULATE REGION      -
CN              VOLUMES.                                                -
CN                                                                      -
CN              DATA ON THIS CARD MAY BE OVERLAYED. THAT IS,            -
CN              TRANSVERSE DISTANCES DEFINED ON LATER TYPE 12           -
CN              CARDS SUPERCEDE DATA FOR REGIONS PREVIOUSLY             -
CN              SPECIFIED.                                              -
CN                                                                      -
CN              IF TYPE 34 CARDS ARE PRESENT, BUCKLINGS WILL BE TAKEN   -
CN              FROM TYPE 34 CARDS AND WILL NOT BE CALCULATED FROM      -
CN              TYPE 12 CARD DATA.  EVEN IF BUCKLINGS ARE TAKEN FROM    -
CN              TYPE 34 CARDS, REGION VOLUMES ARE CALCULATED USING      -
CN              TYPE 12 CARD DATA WHEN TYPE 12 CARDS ARE PRESENT.       -
CN                                                                      -
CN              IN THE ABSENCE OF TYPE 12 AND TYPE 34 CARDS NO          -
CN              BUCKLINGS WILL BE USED AND REGION VOLUMES WILL BE       -
CN              CALCULATED USING UNIT TRANSVERSE HEIGHTS.               -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MATERIAL SPECIFICATIONS (TYPE 13)                           -
C                                                                       -
CL    FORMAT------(I2,10X,A6,3(A6,E12.5))                               -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      13                                                       -
CD                                                                      -
CD    13-18    MATERIAL LABEL (REPEATED ON ADDITIONAL TYPE 13 CARDS).   -
CD                                                                      -
CD    19-24    UNIQUE ISOTOPE LABEL.                                    -
CD                                                                      -
CD    25-36    ISOTOPE ATOM DENSITY (ATOMS/CC * 1.E-24).                -
CD                                                                      -
CD    37-42    UNIQUE ISOTOPE LABEL.                                    -
CD                                                                      -
CD    43-54    ISOTOPE ATOM DENSITY (ATOMS/CC * 1.E-24).                -
CD                                                                      -
CD    55-60    UNIQUE ISOTOPE LABEL.                                    -
CD                                                                      -
CD    61-72    ISOTOPE ATOM DENSITY (ATOMS/CC * 1.E-24).                -
C                                                                       -
CN              MATERIAL LABELS MUST BE NON-BLANK.                      -
CN                                                                      -
CN              MATERIALS CAN BE DEFINED ON A TYPE 13 CARD IN TERMS     -
CN              OF ISOTOPES AND/OR IN TERMS OF OTHER MATERIALS. IN THE  -
CN              LATTER CASE THE "ISOTOPE LABEL" IS A MATERIAL LABEL     -
CN              AND THE "ISOTOPE ATOM DENSITY" IS A VOLUME FRACTION.    -
CN                                                                      -
CN              THE CONCEPT OF MATERIALS DOES NOT EXIST IN THE CCCC     -
CN              ENVIRONMENT, AND THE IDENTITY OF INDIVIDUAL MATERIALS   -
CN              IS LOST WHEN THE CCCC FILES ARE CREATED. TYPE 13        -
CN              CARDS ARE PROVIDED AS AN INPUT CONVENIENCE ONLY.        -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          COMPOSITION SPECIFICATIONS (TYPE 14)                        -
C                                                                       -
CL    FORMAT------(I2,10X,A6,3(A6,E12.5))                               -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      14                                                       -
CD                                                                      -
CD    13-18    COMPOSITION LABEL (REPEATED ON ADDITIONAL TYPE 14        -
CD             CARDS).                                                  -
CD                                                                      -
CD    19-24    MATERIAL LABEL.                                          -
CD                                                                      -
CD    25-36    MATERIAL VOLUME FRACTION.                                -
CD                                                                      -
CD    37-42    MATERIAL LABEL.                                          -
CD                                                                      -
CD    43-54    MATERIAL VOLUME FRACTION.                                -
CD                                                                      -
CD    55-60    MATERIAL LABEL.                                          -
CD                                                                      -
CD    61-72    MATERIAL VOLUME FRACTION.                                -
C                                                                       -
CN              COMPOSITION LABELS MUST BE NON-BLANK.                   -
CN                                                                      -
CN              WHEN A "MATERIAL LABEL" HAS NOT BEEN SPECIFIED          -
CN              (COLS.13-18 OF A TYPE 13 OR TYPE 14 CARD), THE          -
CN              "MATERIAL" WILL BE INTERPRETED AS AN ISOTOPE AND        -
CN              THE "VOLUME FRACTION" WILL BE INTERPRETED AS AN ATOM    -
CN              DENSITY.                                                -
CN                                                                      -
CN              WHEN AN ISOTOPE (OR MATERIAL) IS REFERENCED MORE THAN   -
CN              ONCE FOR A SINGLE COMPOSITION, THE ATOM DENSITIES       -
CN              (OR VOLUME FRACTIONS) ARE SUMMED.                       -
CN                                                                      -
CN              TWO TYPES OF COMPOSITIONS (PRIMARY AND SECONDARY) CAN   -
CN              BE DEFINED ON TYPE 14 CARDS. SECONDARY COMPOSITIONS     -
CN              ARE MIXTURES OF MATERIALS AND/OR ISOTOPES. PRIMARY      -
CN              COMPOSITIONS ARE MIXTURES OF SECONDARY COMPOSITIONS,    -
CN              MATERIALS AND/OR ISOTOPES. ONLY PRIMARY COMPOSITIONS    -
CN              MAY BE ASSIGNED TO REGIONS ON THE TYPE 15 CARDS.        -
CN                                                                      -
CN              SECONDARY COMPOSITIONS ARE TREATED AS CCCC SUBZONES.    -
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CN            THOSE CONSTITUENTS OF A PRIMARY COMPOSITION WHICH ARE -
CN            NOT THEMSELVES SUBZONES (I.E. ISOTOPES AND MATERIALS -
CN            DIRECTLY ASSIGNED TO PRIMARY COMPOSITIONS) ARE       -
CN            COMBINED INTO CCCC PRIMARY ZONE ASSIGNMENTS.         -
CN                                                                 -
CN            AN EXAMPLE OF A SET OF TYPE 13 AND 14 CARDS          -
CN                                                                 -
CN              13  FUEL1 U238   .020   PU239  .003   O16    .042 -
CN              13  FUEL2 U238   .015   PU239  .004   O16    .042 -
CN              13  SS    FE     .055   CR     .015   NI     .012 -
CN              13  COOL  NA23   .022   SS     0.1                -
CN              14  MIX1  FUEL1  1.0                               -
CN              14  MIX2  FUEL1  0.5    FUEL2  0.5                -
CN              14  COMP1 MIX1   0.4    SS     0.2    COOL   0.4 -
CN              14  COMP2 MIX2   0.4    SS     0.2    COOL   0.4 -
CN              14  COMP3 MIX1   0.2    MIX2   0.2    SS     0.2 -
CN              14  COMP3 COOL   0.2                               -
CN              14  COMP4 NA23   .022                              -
CN                                                                 -
CN                  THE MATERIAL COOL IS DEFINED IN TERMS OF AN    -
CN                  ISOTOPE (NA23) AND A MATERIAL (SS).            -
CN                                                                 -
CN                  MIX1 AND MIX2 ARE SECONDARY COMPOSITIONS.      -
CN                  COMP1, COMP2, COMP3 AND COMP4 ARE PRIMARY      -
CN                  COMPOSITIONS.                                  -
CN                                                                 -
CN                  IN THE CCCC FILES MIX1 WILL BE ASSIGNED AS     -
CN                  SUBZONES TO BOTH COMP1 AND COMP3. THE PRIMARY  -
CN                  ZONE ASSIGNMENTS OF COMP1, COMP2 AND COMP3     -
CN                  WILL CONSIST OF SS AND COOL. COMP4 WILL HAVE   -
CN                  NO SUBZONES.                                   -
C                                                                  -
C------------------------------------------------------------------

C------------------------------------------------------------------
CR          ASSIGNMENT OF REGION TO COMPOSITION (CCCC ZONE)        -
CR          (TYPE 15)                                              -
C                                                                  -
CL    FORMAT------(I2,4X,11A6)                                     -
C                                                                  -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY             -
CD    -------  ------------------------------------------------    -
CD    1-2      15                                                  -
CD                                                                 -
CD    7-12     COMPOSITION (CCCC ZONE) LABEL (REPEATED ON ADDITIONAL -
CD             TYPE 15 CARDS).                                     -
CD                                                                 -
CD    13-18    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    19-24    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    25-30    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    31-36    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    37-42    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    43-48    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    49-54    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    55-60    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    61-66    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
CD                                                                 -
CD    67-72    REGION LABEL OR AREA LABEL DEFINING REGION(S)       -
CD             CONTAINING SPECIFIED COMPOSITION.                   -
C                                                                  -
CN            AN AREA LABEL IN COLS. 13-72 IMPLIES ALL THE REGIONS -
CN            ASSIGNED TO THAT AREA.  AREAS ARE DEFINED ON THE     -
CN            TYPE 07 CARD.                                        -
CN                                                                 -
CN            WHEN A PARTICULAR REGION OR AREA IS REFERENCED ON    -
CN            MORE THAN ONE TYPE 15 CARD, THE LAST REFERENCE       -
CN            TO THAT REGION (EITHER DIRECTLY, OR THROUGH AN AREA) -
CN            ESTABLISHES THE COMPOSITION ASSIGNMENT.              -
CN            I.E. A REGION/COMPOSITION CORRESPONDENSE ESTABLISHED -
CN            ON ONE TYPE 15 CARD CAN BE OVERWRITTEN BY A          -
CN            REFERENCE ON A LATER TYPE 15 CARD.                   -
CN                                                                 -
CN            COMPOSITION LABELS MUST BE NON-BLANK.  THE FIRST     -
CN            BLANK REGION LABEL ENCOUNTERED TERMINATES READING    -
CN            OF THE DATA ON THAT PARTICULAR TYPE 15 CARD.         -
CN                                                                 -
CN            ONLY PRIMARY COMPOSITION LABELS (SEE CARD TYPE 14)   -
CN            CAN APPEAR IN COLS. 7-12. PRIMARY COMPOSITIONS ARE   -
CN            EQUIVALENT TO CCCC ZONES. A REGION CAN CONTAIN ONLY  -
CN            ONE PRIMARY COMPOSITION.                             -
CN                                                                 -
CN            WHEN THERE ARE NO TYPE 14 CARDS (THE MACROSCOPIC     -
CN            CROSS SECTIONS ALREADY EXIST) THE COMPOSITION        -
CN            LABEL FIELDS SHOULD CONTAIN COMPOSITION NUMBERS      -
CN            INSTEAD (I2,4X,I6,10A6).                             -
C                                                                  -
C------------------------------------------------------------------

C------------------------------------------------------------------
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CR        DISTRIBUTED ISOTROPIC INHOMOGENEOUS SOURCE DATA DEFINED
CR        EITHER BY REGION OR MESH INTERVAL (TYPE 19)
C
CL    FORMAT------(I2,4X,A6,2I6,4E12.5)
C
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======  ==================================================
CD    1-2      19
CD
CD    7-12     LABEL OF REGION OR AREA (BLANK IF DATA ARE GIVEN BY
CD             MESH INTERVALS).  IF THE GEOMETRY HAS BEEN SPECIFIED
CD             BY AN INPUT GEODST FILE (AND NOT BY A.NIP TYPE 06
CD             OR 30 CARDS) USE THE REGION NUMBER (I6) INSTEAD OF
CD             THE REGION LABEL.
CD
CD    13-18    HIGHER-ENERGY GROUP NUMBER.
CD
CD    19-24    LOWER-ENERGY GROUP NUMBER.
CD
CD    25-36    ISOTROPIC SOURCE VALUE IN THE SPECIFIED MESH INTERVAL,
CD             REGION OR AREA FOR THIS ENERGY RANGE.  (NEUTRONS PER
CD             SECOND PER UNIT VOLUME).
CD
CD    37-48    LOWER "X" DIRECTION COORDINATE OF MESH INTERVAL
CD             CONTAINING THIS SOURCE.
CD
CD    49-60    LOWER "Y" DIRECTION COORDINATE OF MESH INTERVAL
CD             CONTAINING THIS SOURCE.
C
CD    61-72    LOWER Z DIRECTION COORDINATE OF MESH INTERVAL
CD             CONTAINING THIS SOURCE.
CD
CN             AN AREA LABEL IN COLS. 7-12 IMPLIES ALL THE REGIONS
CN             ASSIGNED TO THAT AREA.
CN
CN             IF THERE IS NO REGION LABEL (COLS. 7-12 ARE BLANK),
CN             THE SOURCE SPECIFIED IN COLS. 25-36 IS PLACED IN THE
CN             MESH BOX DEFINED BY COLS. 37-48, 49-60 AND 61-72.
CN
CN             IF THERE IS A REGION LABEL (COLS. 7-12 ARE NON-BLANK),
CN             THE MESH COORDINATE FIELDS (COLS. 37-48, 49-60 AND
CN             61-72) ARE IGNORED AND THE SOURCE SPECIFIED IN COLS.
CN             25-36 IS PLACED IN EVERY MESH BOX IN THE REGION.
CN
CN             "X" REPRESENTS THE FIRST DIMENSION COORDINATE (X IN
CN             X-Y GEOMETRY, R IN R-Z, ETC.).  "Y" REPRESENTS THE
CN             SECOND DIMENSION COORDINATE (Y IN X-Y GEOMETRY, Z IN
CN             R-Z, ETC.).  WHEN THE MODEL IS THREE-DIMENSIONAL, THE
CN             THIRD DIMENSION IS ALWAYS Z.
C
CN             IN GEOMETRIES INVOLVING AN ANGULAR DIMENSION (THETA)
CN             THE ANGULAR VARIABLE MUST BE GIVEN IN RADIANS.
CN
CN             IF NO "HIGHER-ENERGY GROUP NUMBER" IS SUPPLIED (COLS.
CN             13-18 ARE BLANK), THE SOURCE VALUE GIVEN APPLIES TO
CN             ALL ENERGY GROUPS.  IF NO "LOWER-ENERGY GROUP NUMBER"
CN             IS SUPPLIED (COLS. 19-24 ARE BLANK), THE SOURCE VALUE
CN             GIVEN APPLIES TO THE "HIGHER-ENERGY GROUP" ONLY.  IF
CN             NO GROUP NUMBERS ARE SUPPLIED (COLS. 13-24 ARE BLANK),
CN             THE SOURCE VALUE GIVEN APPLIES TO ALL ENERGY GROUPS.
CN
CN             DATA ON THIS CARD MAY BE OVERLAYED.  THAT IS, SOURCE
CN             VALUES DEFINED ON LATER TYPE 19 CARDS SUPERCEDE DATA
CN             FOR REGIONS AND GROUPS PREVIOUSLY SPECIFIED.
CN
CN             AN EDIT OF THE OUTPUT FIXSRC FILE MAY BE OBTAINED BY
CN             SUPPLYING THE EDIT SENTINEL ON THE TYPE 40 CARD.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          SEARCH EDIT OPTIONS AND CONVERGENCE CRITERIA (TYPE 21)
C
CL    FORMAT------(I2,10X,2I6,2E12.5,2I6)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======  ==================================================
CD    1-2      21
CD
CD    13-18    SEARCH FILE PROCESSING EDIT SENTINEL
CD                 0, NO EDITS (DEFAULT).
CD                 1, PRINT EDITS.
CD                 2, WRITE EDITS TO AUXILIARY OUTPUT FILE.
CD                 3, WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT
CD                    FILE.
CD
CD    19-24    MAXIMUM NUMBER OF SEARCH PASSES (DEFAULT=4).
CD
CD    25-36    DESIRED KEFF, KEFF(0) (DEFAULT=1.0).
CD
CD    37-48    CONVERGENCE CRITERION, EPSILON: RELATIVE ERROR BOUND
CD             FOR KEFF (DEFAULT=.01).
CD
CD             ABSOLUTE VALUE OF ((KEFF-KEFF(0)) / KEFF(0)).LE.
CD             EPSILON.
CD
CD    49-54    SEARCH (MODULE) PARAMETER EDIT OPTIONS
CD             ENTER TWO-DIGIT NUMBER (IF) WHERE
CD
CD             I CONTROLS INTERMEDIATE PASS PARAMETER EDITS
CD             F CONTROLS FINAL SEARCH PASS PARAMETER EDITS
CD
CD             THE INTEGERS I AND F ARE ASSIGNED ONE OF THE
CD             FOLLOWING VALUES (LEADING ZEROES ARE IRRELEVANT)
CD             0...NO EDITS
CD             1...PRINT EDITS (DEFAULT FOR F)
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CD            2...WRITE EDITS TO AUXILIARY OUTPUT FILE                -
CD            3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
CD                                                                    -
CD    55-60   SEARCH (MODULE) QUANTITY EDIT OPTIONS                  --
CD            ENTER TWO-DIGIT NUMBER (IF) WHERE                       -
CD                                                                    -
CD            I CONTROLS INTERMEDIATE PASS QUANTITY EDITS             -
CD            F CONTROLS FINAL SEARCH PASS QUANTITY EDITS             -
CD                                                                    -
CD            THE INTEGERS I AND F ARE ASSIGNED ONE OF THE            -
CD            FOLLOWING VALUES (LEADING ZEROES ARE IRRELEVANT)        -
CD            0...NO EDITS (DEFAULT)                                  -
CD            1...PRINT EDITS                                         -
CD            2...WRITE EDITS TO AUXILIARY OUTPUT FILE                -
CD            3...WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT FILE-
C                                                                     -
CN            EACH SEARCH PASS REQUIRES THE SUCCESSFUL COMPLETION     -
CN            OF AN EIGENVALUE PROBLEM BY A NEUTRONICS MODULE.        -
CN            SUCCESSFUL NEUTRONICS MODULE COMPLETION IS INDICATED BY-
CN              1.  OUTER ITERATIONS CONVERGED OR                     -
CN              2.  MAXIMUM NUMBER OF OUTER ITERATIONS ATTAINED.      -
C                                                                     -
CN            NONZERO DATA ON THIS CARD OVERRIDES DATA IN AN EXISTING-
CN            SEARCH FILE DURING A SEARCH PROBLEM RESTART.             -
C                                                                     -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          SEARCH PARAMETER DATA (TYPE 22)                           -
C                                                                     -
CL    FORMAT-----(I2,10X,5E12.5)                                      -
C                                                                     -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD    =======  ==========================================================-
CD    1-2      22                                                      -
CD                                                                    -
CD    13-24    INITIAL ESTIMATE OF X (DEFAULT=0.0).                    -
CD                                                                    -
CD    25-36    SECOND ESTIMATE OF X (IGNORED IF COLS. 61-72 ARE        -
CD             NON-ZERO) (DEFAULT=0.1 (X=0.0), =1.1*X (X NE 0.0))      -
CD                                                                    -
CD    37-48    LOWER BOUND FOR X (DEFAULT=0.0).                        -
CD                                                                    -
CD    49-60    UPPER BOUND FOR X (DEFAULT=1.0).                        -
CD                                                                    -
CD    61-72    DERIVATIVE OF KEFF WITH RESPECT TO X (OPTIONAL).        -
CN             (PROVIDES AN ALTERNATE METHOD FOR OBTAINING SECOND      -
CN             ESTIMATE OF X IN COLS. 25-36).                          -
C                                                                     -
CN             COLS. 25-36 ARE IGNORED IF COLS. 61-72 CONTAIN OTHER    -
CN             THAN BLANK OR 0.0.                                      -
CN                                                                    -
CN             GENERAL SEARCH EXPRESSION:  P(X) = P(0) + X * M,        -
CN             WHERE P IS THE QUANTITY BEING VARIED, X IS THE SEARCH   -
CN             PARAMETER, AND M IS THE QUANTITY MODIFIER OBTAINED      -
CN             FROM INFORMATION CONTAINED ON ONE OF THE MUTUALLY       -
CN             EXCLUSIVE CARD TYPES 23, 24, 25, OR 26.  X IS TO BE     -
CN             VARIED UNTIL THE DESIRED KEFF IS REACHED.  THE SEARCH   -
CN             WILL BE TERMINATED IF X EXCEEDS ITS BOUNDS OR IF THE    -
CN             MAXIMUM NUMBER OF SEARCH PASSES ARE REACHED.            -
CN             (SOME CODES MAY ALSO TRIGGER JOB TERMINATION BETWEEN    -
CN             SEARCH PASSES IF IT IS ESTIMATED THAT JOB TIME LIMIT    -
CN             WOULD BE EXCEEDED DURING THE NEXT SEARCH PASS).         -
CN                                                                    -
CN             FOR EFFICIENT SEARCHING, SCALE THE SEARCH QUANTITY      -
CN             SUCH THAT THE MAGNITUDES OF THE SEARCH PARAMETER        -
CN             ESTIMATES LIE IN THE INTERVAL (.1,10.)                  -
CN                                                                    -
CN             NONZERO DATA ON THIS CARD OVERRIDES DATA IN AN EXISTING-
CN             SEARCH FILE DURING A SEARCH PROBLEM RESTART.             -
C                                                                     -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          CONCENTRATION MODIFIERS FOR CRITICALITY SEARCH (TYPE 23)   -
C                                                                     -
CL    FORMAT-----(I2,4X,11A6)                                         -
C                                                                     -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD    =======  ==========================================================-
CD    1-2      23                                                      -
CD                                                                    -
CD    7-12     COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO BE USED AS THE MODIFIER M IN THE SEARCH FORMULA.     -
CD                                                                    -
CD    13-18    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
CD    19-24    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
CD    25-30    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
CD    31-36    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
CD    37-42    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
CD    43-48    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
CD    49-54    COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)    -
CD             TO WHICH MODIFIER M IS ADDED AS A SUBZONE.              -
CD                                                                    -
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CD    55-60     COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)  -
CD              TO WHICH MODIFIER M IS ADDED AS A SUBZONE.            -
CD                                                                    -
CD    61-66     COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)  -
CD              TO WHICH MODIFIER M IS ADDED AS A SUBZONE.            -
CD                                                                    -
CD    67-72     COMPOSITION LABEL OF COMPOSITION (FROM CARD TYPE 14)  -
CD              TO WHICH MODIFIER M IS ADDED AS A SUBZONE.            -
C                                                                     -
CN              IN THE SEARCH FORMULA  P(X) = P(0) + X * M,           -
CN              P(0) DENOTES THOSE PRIMARY COMPOSITIONS (ZONES,       -
CN              COLS. 13-72) TO WHICH THE MODIFIER COMPOSITIONS (M,   -
CN              COLS. 7-12) ARE ADDED AS SUBZONES,                    -
CN              X IS THE VOLUME FRACTION APPLIED TO THE MODIFIER      -
CN              COMPOSITIONS (CCCC ZONES OR SUBZONES) COMPRISING M,   -
CN              AND P(X) DENOTES THE RESULTANT COMPOSITIONS.          -
CN              CARD TYPE 23 DEFINES P(0) AND M IN TERMS OF COMPOSITION-
CN              LABELS DEFINED ON CARD TYPE 14.                       -
CN                                                                    -
CN              THE MODIFIER COMPOSITION (CCCC ZONE OR SUBZONE) NAME  -
CN              IN COLS. 7-12 MUST BE A SUBZONE OR AN UNASSIGNED (NOT -
CN              ASSIGNED TO A REGION ON A TYPE 15 CARD) PRIMARY ZONE  -
CN              CONTAINING NO SUBZONES.                               -
CN                                                                    -
CN              THE MODIFIER COMPOSITIONS (M) BECOME SUBZONES OF      -
CN              EACH ZONE SPECIFIED IN COLS. 13-72.  WHEN A SUBZONE IS -
CN              SPECIFIED IN COLS 13-72, THE MODIFIER COMPOSITIONS (M) -
CN              BECOME SUBZONES IN EACH ZONE CONTAINING THE SUBZONE   -
CN              IN COLS. 13-72.  IN BOTH CASES THE VOLUME FRACTION    -
CN              OF THE ADDED SUBZONES IS X.                           -
CN                                                                    -
CN              A MODIFIER COMPOSITION (M) CANNOT MODIFY ANOTHER      -
CN              MODIFIER COMPOSITION OR A COMPOSITION WHICH ALREADY   -
CN              CONTAINS THE MODIFIER COMPOSITION AS A ZONE OR SUBZONE.-
CN                                                                    -
CN              AN EXAMPLE OF A SET OF TYPE 23 CARDS USING THE SAMPLE -
CN              TYPE 14 CARDS PRESENTED IN THE TYPE 14 CARD DESCRIPTION-
CN              FOLLOWS:                                              -
CN                                                                    -
CN                23  COMP4 COMP1 MIX2                                -
CN                23  MIX1  COMP2                                     -
CN                                                                    -
CN                    IN THE CCCC FILES COMP4 WILL BECOME A SUBZONE   -
CN                    OF COMP1, COMP2 AND COMP3.  MIX1 WILL BECOME    -
CN                    A SUBZONE OF COMP2.                             -
CN                                                                    -
CN              REPEAT TYPE 23 CARDS AS NEEDED.                       -
C                                                                     -
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          MESH MODIFIERS FOR CRITICALITY SEARCH (TYPE 24)           -
C                                                                     -
CL    FORMAT-----(I2,9X,A1,3E12.5)                                    -
C                                                                     -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD    =======  ========================================================-
CD    1-2      24                                                     -
CD                                                                    -
CD    12       COORDINATE DIRECTION.                                  -
CD             X..."X" COORDINATE DIRECTION.                          -
CD             Y..."Y" COORDINATE DIRECTION.                          -
CD             Z..."Z" COORDINATE DIRECTION.                          -
CD                                                                    -
CD    13-24    LOWER (COARSE MESH) COORDINATE.                        -
CD                                                                    -
CD    25-36    UPPER (COARSE MESH) COORDINATE.                        -
CD                                                                    -
CD    37-48    MESH MODIFIER, M, FOR EACH MESH INTERVAL BETWEEN       -
CD             THE ABOVE COORDINATES.                                 -
C                                                                     -
CN             IN THE SEARCH FORMULA P(X) = P(0) + X * M,             -
CN             P(X) IS THE RESULTING MESH INTERVAL,                   -
CN             P(0) IS THE INITIAL MESH INTERVAL, AND                 -
CN             M IS THE MESH INTERVAL MODIFIER.                       -
CN                                                                    -
CN             DATA ON THIS CARD MAY BE OVERLAYED.  THAT IS MESH      -
CN             MODIFIERS DEFINED ON LATER TYPE 24 CARDS SUPERCEDE     -
CN             DATA FOR REGIONS SPECIFIED PREVIOUSLY.                 -
CN                                                                    -
CN             REPEAT TYPE 24 CARDS AS NEEDED.                        -
C                                                                     -
C---------------------------------------------------------------------

C---------------------------------------------------------------------
CR          COMPOSITION DEPENDENT BUCKLING MODIFIERS FOR CRITICALITY   -
CR          SEARCH (TYPE 25)                                          -
C                                                                     -
CL    FORMAT-----(I2,4X,A6,E12.5)                                     -
C                                                                     -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                -
CD    =======  ========================================================-
CD    1-2      25                                                     -
CD                                                                    -
CD    7-12     COMPOSITION (ZONE) LABEL.                              -
CD                                                                    -
CD    13-24    BUCKLING MODIFIER, M, IN FIRST TRANSVERSE DIRECTION.   -
C                                                                     -
CD    25-36    BUCKLING MODIFIER, M, IN SECOND TRANSVERSE DIRECTION   -
CD             FOR A FINITE ONE-DIMENSIONAL RECTANGULAR SLAB.         -
C                                                                     -
CN             IN THE SEARCH FORMULA  P(X) = P(0) + X * M,            -
CN             P(X) IS THE RESULTING BUCKLING, P(0) IS THE INITIAL    -
CN             BUCKLING, AND M IS THE BUCKLING MODIFIER.              -
CN             P(0) WILL BE EVALUATED FROM THE TRANSVERSE HEIGHTS     -
CN             GIVEN ON CARD TYPE 12 OR TAKEN DIRECTLY FROM BUCKLINGS -
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CN              GIVEN ON CARD TYPE 34.                                  -
CN                                                                      -
CN              IF COLS. 7-12 ARE BLANK, THE DATA IN COLS. 13-24 APPLY  -
CN              TO ALL COMPOSITIONS (ZONES) OF THE REACTOR.             -
CN                                                                      -
CN              REPEAT TYPE 25 CARDS AS NEEDED.                         -
C                                                                       -
C-----------------------------------------------------------------------
```

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C-----------------------------------------------------------------------
CR          ALPHA MODIFIER FOR CRITICALITY SEARCH (TYPE 26)              -
C                                                                       -
CL    FORMAT-----(I2,10X,E12.5)                                         -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    -------  ------------------------------------------------------  -
CD    1-2      26                                                       -
CD                                                                      -
CD    13-24    ALPHA MODIFIER, M.                                       -
CD                                                                      -
C                                                                       -
CN              IN THE SEARCH FORMULA  P(X) = P(0) + X * M,             -
CN              P(X) IS THE RESULTING ALPHA, P(0) IS THE INITIAL ALPHA, -
CN              AND M IS THE ALPHA MODIFIER.                            -
C                                                                       -
C-----------------------------------------------------------------------
```

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C-----------------------------------------------------------------------
CR          HEXAGON DIMENSION (TYPE 29)                                 -
C                                                                       -
CL    FORMAT-----(I2,10X,E12.5,2I6)                                     -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    -------  ------------------------------------------------------  -
CD    1-2      29                                                       -
CD                                                                      -
CD    13-24    DIMENSION OF HEXAGON ACROSS FLATS.                       -
CD                                                                      -
CD    25-30    TOTAL NUMBER OF HEXAGONAL RINGS IN THE REGION OF         -
CD             SOLUTION.                                                -
CD                                                                      -
CD    31-36    FOR TRIANGULAR AND TRIANGULAR-Z GEOMETRIES, THE          -
CD             NUMBER OF EQUAL PARTS INTO WHICH EACH SIDE OF THE        -
CD             BASIC EQUILATERAL TRIANGLES MAKING UP THE HEXAGONS ARE   -
CD             SUBDIVIDED.  THUS E.G., IF COLS 31-36 CONTAIN 3, THE     -
CD             HEXAGON CONTAINS 54 MESH POINTS INSTEAD OF THE NORMAL    -
CD             6.                                                       -
C                                                                       -
CN              IF THE NUMBER OF RINGS IS NOT PROVIDED IN COLS. 25-30,  -
CN              IT IS DERIVED FROM THE TYPE 30 CARDS.                   -
CN                                                                      -
CN              IF COLS. 31-36 ARE BLANK, THE TRIANGLES ARE NOT         -
CN              SUBDIVIDED.                                             -
CN                                                                      -
CN              THE TYPE 29 CARD IS PERTINENT ONLY IF COLS. 13-18 ON    -
CN              CARD TYPE 03 ARE GREATER THAN OR EQUAL TO 70.           -
CN                                                                      -
CN              FOR TRIANGULAR-Z AND HEXAGONAL-Z GEOMETRIES THE         -
CN              AXIAL (Z) MESH MUST BE SPECIFIED ON TYPE 9 CARDS.       -
C                                                                       -
C-----------------------------------------------------------------------
```

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C-----------------------------------------------------------------------
CR          LOCATIONS OF REGIONS FOR TRIANGULAR, TRIANGULAR-Z,          -
CR          HEXAGONAL, AND HEXAGONAL-Z GEOMETRIES (TYPE 30)             -
C                                                                       -
CL    FORMAT-----(I2,4X,A6,3I6,2E12.5)                                  -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    -------  ------------------------------------------------------  -
CD    1-2      30                                                       -
CD                                                                      -
CD    7-12     REGION LABEL (REPEATED ON ADDITIONAL TYPE 30 CARDS).     -
CD                                                                      -
CD    13-18    HEXAGONAL RING NUMBER WHERE REGION IS LOCATED.           -
CD                                                                      -
CD    19-24    STARTING HEXAGON POSITION FOR THIS REGION.               -
CD                                                                      -
CD    25-30    FINAL HEXAGON POSITION FOR THIS REGION.                  -
CD                                                                      -
CD    31-42    LOWER Z BOUNDARY OF REGION.                              -
CD                                                                      -
CD    43-54    UPPER Z BOUNDARY OF REGION.                              -
CD                                                                      -
C                                                                       -
CN              REGION LABELS MUST BE NON-BLANK.                        -
CN                                                                      -
CN              IF THE STARTING POSITION (COLS. 19-24) IS BLANK OR      -
CN              ZERO, THE REGION LABEL IS ASSIGNED TO THE WHOLE RING.   -
CN                                                                      -
CN              IF THE FINAL POSITION (COLS. 25-30) IS BLANK OR ZERO,   -
CN              THE REGION LABEL IS ASSIGNED TO THE POSITION IN 19-24   -
CN              OF THE RING IN 13-18.                                   -
CN                                                                      -
CN              DATA ON THIS CARD MAY BE OVERLAYED. THAT IS, REGION     -
CN              ASSIGNMENTS DEFINED ON LATER TYPE 30 CARDS SUPERCEDE    -
CN              DATA FOR RINGS AND POSITIONS PREVIOUSLY SPECIFIED.      -
CN                                                                      -
CN              THE REGION LOWER AND UPPER Z BOUNDARIES MUST COINCIDE   -
CN              WITH MESH LINES, WHICH BOUND MESH INTERVALS.            -
CN                                                                      -
CN              THE FIGURE BELOW ILLUSTRATES THE ORDER OF NAMING        -
CN              RINGS AND HEXAGONS IN THE RINGS.  THE FIRST NUMBER OF   -
CN              EACH NUMBERED PAIR IS THE RING NUMBER, AND THE SECOND   -
CN              NUMBER IS THE HEXAGON NUMBER IN THAT RING.              -
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CN              THE REGION OF SOLUTION DEPENDS ON THE VALUE IN COLS.   -
CN              13-18 ON CARD TYPE 03 AS FOLLOWS.                       -
CN                                                                      -
CN        COLS. 13-18 ON CARD TYPE 03       REGION OF SOLUTION          -
CN        ===========================    ==========================     -
CN                  80                    ENTIRE FIGURE AS SHOWN BELOW  -
CN                  72                    IN THE 180 DEGREE SECTOR A-B  -
CN                  78                    IN THE 90 DEGREE SECTOR A-C   -
CN                  70                    IN THE 60 DEGREE SECTOR A-D   -
CN                  74                    IN THE 120 DEGREE SECTOR A-E  -
CN                  110                   ENTIRE FIGURE AS SHOWN BELOW  -
CN                  114                   IN THE 60 DEGREE SECTOR F-C   -
CN                  116                   IN THE 120 DEGREE SECTOR F-G  -
CN                                                                      -
CN                    G             E             C                     -
CN                                                                      -
CN                      *           *           *                       -
CN                                                                      -
CN       B                *         *         *                         -
CN          *                                                     D     -
CN             *            *       *       *                 *         -
CN                *         ====== ====== ======           *            -
CN                   *      =3,5 = =3,4 = =3,3 =        *               -
CN                      *   ====== ====== ======     *                  -
CN                       ====== ====== ====== ======                    -
CN                       =3,6 = =2,3 = =2,2 = =3,2 =                    -
CN                       ====== ====== ====== ======                    -
CN                    ====== ====== ====== ====== ======                -
CN                    =3,7 = =2,4 = =1,1 = =2,1 = =3,1 =  *  *  *  F    -
CN                    ====== ====== ====== ====== ======                -
CN                       ====== ====== ====== ======                    -
CN                       =3,8 = =2,5 = =2,6 = =3,12=                    -
CN                       ====== ====== ====== ======                    -
CN                          ====== ====== ======     *                  -
CN                          =3,9 = =3,10= =3,11=        *               -
CN                          ====== ====== ======           *            -
CN                                                            *         -
CN                                                               A      -
CN                                                                      -
CN                                                                      -
CN              ALTHOUGH THE REGIONS OF SOLUTION DIFFER FOR THE         -
CN              TRIANGULAR AND HEXAGONAL GEOMETRY MODELS, TYPE 30       -
CN              CARDS COMPOSED FOR TRIANGULAR GEOMETRY MODELS CAN ALSO  -
CN              BE USED FOR HEXAGONAL GEOMETRY MODELS.                  -
CN                                                                      -
C                                                                       -
C------------------------------------------------------------------------
```

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C------------------------------------------------------------------------
CR          BACKGROUND REGION NAME FOR TRIANGULAR, TRIANGULAR-Z,        -
CR          HEXAGONAL, AND HEXAGONAL-Z GEOMETRIES (TYPE 31)             -
C                                                                       -
CL    FORMAT-----(I2,4X,A6)                                             -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======   ==================================================------
CD    1-2       31                                                      -
CD                                                                      -
CD    7-12      BACKGROUND REGION NAME.                                 -
C                                                                       -
CN              ANY PORTION OF THE REACTOR NOT SPECIFIED ON THE         -
CN              TYPE 30 CARDS WILL BE IN THE BACKGROUND REGION.         -
CN                                                                      -
CN              IF THE BACKGROUND REGION NAME (COLS. 7-12) IS BLANK,    -
CN              OR IF THERE IS NO TYPE 31 CARD, THE BACKGROUND REGION   -
CN              WILL BE ASSIGNED A REGION NUMBER 0 (ZERO).  NOTE THAT   -
CN              SOME CCCC CODES EXCLUDE SUCH A REGION FROM THE REGION   -
CN              OF SOLUTION, WHILE OTHER CCCC CODES MAY NOT ALLOW       -
CN              ZERO REGION NUMBERS.                                    -
C                                                                       -
C------------------------------------------------------------------------
```

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C------------------------------------------------------------------------
CR          COMPOSITION AND GROUP DEPENDENT BUCKLING SPECIFICATIONS     -
CR          (TYPE 34)                                                   -
C                                                                       -
CL    FORMAT-----(I2,4X,A6,2(E12.5,2I6))                                -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======   =========================================================
CD    1-2       34                                                      -
CD                                                                      -
CD    7-12      COMPOSITION LABEL.                                      -
CD                                                                      -
CD    13-24     BUCKLING (B**2).                                        -
CD                                                                      -
CD    25-30     HIGHER ENERGY BROAD GROUP NUMBER TO WHICH BUCKLING      -
CD              IN COLS. 13-24 APPLIES.                                 -
CD                                                                      -
CD    31-36     LOWER ENERGY BROAD GROUP NUMBER TO WHICH BUCKLING       -
CD              IN COLS. 13-24 APPLIES.                                 -
CD                                                                      -
CD    37-48     BUCKLING (B**2).                                        -
CD                                                                      -
CD    49-54     HIGHER ENERGY BROAD GROUP NUMBER TO WHICH BUCKLING      -
CD              IN COLS. 37-48 APPLIES.                                 -
CD                                                                      -
CD    55-60     LOWER ENERGY BROAD GROUP NUMBER TO WHICH BUCKLING       -
CD              IN COLS. 37-48 APPLIES.                                 -
C                                                                       -
CN              IF THERE IS NO COMPOSITION LABEL (COLS. 7-12 ARE        -
CN              BLANK), THE BUCKLINGS ON THIS CARD WILL APPLY TO        -
CN              ALL COMPOSITIONS.                                       -
CN                                                                      -
CN              IF NO "HIGHER-ENERGY GROUP NUMBER" IS SUPPLIED IN       -
CN              COLS. 25-30, THE BUCKLING GIVEN IN COLS. 13-24 APPLIES  -
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CD              TO ALL ENERGY GROUPS.  IF THERE IS A "HIGHER-ENERGY     -
CD              GROUP NUMBER" IN COLS. 25-30, BUT NO "LOWER-ENERGY      -
CD              GROUP NUMBER" IS SUPPLIED IN COLS. 31-36, THE BUCKLING  -
CD              GIVEN IN COLS. 13-24 APPLIES TO THE "HIGHER-ENERGY      -
CD              GROUP" ONLY.                                            -
CN                                                                      -
CN              IF NO "HIGHER-ENERGY GROUP NUMBER" IS SUPPLIED IN       -
CN              COLS. 49-54, THE DATA IN COLS. 37-60 ARE IGNORED. IF    -
CN              THERE IS A "HIGHER-ENERGY GROUP NUMBER" IN COLS. 49-54, -
CN              BUT NO "LOWER-ENERGY GROUP NUMBER" IN COLS. 55-60,      -
CN              THE BUCKLING GIVEN IN COLS. 37-48 APPLIES TO THE        -
CN              "HIGHER-ENERGY GROUP" ONLY.                             -
CN                                                                      -
CN              BUCKLINGS CAN BE OVERLAYED. THAT IS, BUCKLINGS DEFINED  -
CN              ON LATER TYPE 34 CARDS SUPERCEDE DATA FOR COMPOSITIONS  -
CN              AND/OR ENERGY RANGES PREVIOUSLY DEFINED. THE EXCEPTION  -
CN              TO THIS RULE IS THE SITUATION DESCRIBED IN THE PRE-     -
CN              CEDING PARAGRAPHS WHERE DATA IS SPECIFICALLY IGNORED.   -
CN                                                                      -
CN              EXAMPLE         34    **  .001  1  3  .002  4  7       -
CN                              34    COMP1  .003  1  5                 -
CN                              34    COMP1  .004  3                    -
CN                              34    COMP2  .005                       -
CN                                                                      -
CN              THIS EXAMPLE IS IN FREE-FORMAT - ** IMPLIES A BLANK     -
CN              LABEL.  COMPOSITION COMP1 IS BUCKLED .003 IN GROUPS     -
CN              1-2, .004 IN GROUP 3, .003 IN GROUPS 4-5, .002 IN       -
CN              GROUPS 6-7, AND ZERO IN ALL OTHER GROUPS.               -
CN              COMPOSITION COMP2 IS BUCKLED .005 IN ALL GROUPS.  ALL   -
CN              OTHER COMPOSITIONS ARE BUCKLED .001 IN GROUPS 1-3,      -
CN              .002 IN GROUPS 4-7 AND ZERO IN ALL OTHER GROUPS.        -
CN                                                                      -
CN              WHEN ANY TYPE 34 CARDS EXIST, BUCKLINGS WILL NOT BE     -
CN              CALCULATED FROM FINITE GEOMETRY DATA ON TYPE 12 CARDS.  -
C                                                                       -
C-----------------------------------------------------------------------
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C-----------------------------------------------------------------------
CR          DIRECTIONAL DIFFUSION COEFFICIENT FACTOR SCHEME (TYPE 35)   -
C                                                                       -
CL      FORMAT------(I2,4X,A6,6F6.2,2I6)                               -
C                                                                       -
CD      COLUMNS           CONTENTS...IMPLICATIONS, IF ANY               -
CD      -------  ------------------------------------------------------
CD      1-2       35                                                    -
CD                                                                      -
CD      7-12      DIRECTIONAL DIFFUSION COEFFICIENT FACTOR SCHEME LABEL. -
CD                                                                      -
CD      13-18     FIRST DIMENSION DIFFUSION COEFFICIENT MULTIPLIER, A1.  -
CD                                                                      -
CD      19-24     FIRST DIMENSION DIFFUSION COEFFICIENT ADDITIVE         -
CD                TERM, B1.                                             -
CD                                                                      -
CD      25-30     SECOND DIMENSION DIFFUSION COEFFICIENT MULTIPLIER, A2. -
CD                                                                      -
CD      31-36     SECOND DIMENSION DIFFUSION COEFFICIENT ADDITIVE        -
CD                TERM, B2.                                             -
CD                                                                      -
CD      37-42     THIRD DIMENSION DIFFUSION COEFFICIENT MULTIPLIER, A3.  -
CD                                                                      -
CD      43-48     THIRD DIMENSION DIFFUSION COEFFICIENT ADDITIVE         -
CD                TERM, B3.                                             -
CD                                                                      -
CD      49-54     HIGHER ENERGY BROAD GROUP NUMBER TO WHICH DATA IN      -
CD                COLS. 13-48 APPLY.                                    -
CD                                                                      -
CD      55-60     LOWER ENERGY BROAD GROUP NUMBER TO WHICH DATA IN       -
CD                COLS. 13-48 APPLY.                                    -
C                                                                       -
CN              IF MORE THAN ONE TYPE 35 CARD IS NEEDED FOR A GIVEN     -
CN              DIFFUSION COEFFICIENT FACTOR SCHEME, THE LABEL IN       -
CN              COLS. 7-12 MUST BE REPEATED ON EACH ADDITIONAL CARD.    -
CN                                                                      -
CN              FIRST, SECOND AND THIRD DIMENSIONS REFER TO THE         -
CN              DIMENSIONS IN THE ORDER THEY ARE NAMED ON CARD TYPE 3.  -
CN              E.G. FOR R-Z GEOMETRY R IS THE FIRST DIMENSION, AND     -
CN              Z IS THE SECOND.                                        -
CN                                                                      -
CN              THE FIRST DIMENSION DIFFUSION COEFFICIENT, D1, IS       -
CN              CALCULATED FROM THE HOMOGENEOUS DIFFUSION COEFFICIENT,  -
CN              D, AS FOLLOWS:                                          -
CN                                                                      -
CN                                      D1 = A1*D+B1                    -
CN                                                                      -
CN              THE OTHER TWO DIMENSIONS ARE HANDLED IN A SIMILAR WAY.  -
CN                                                                      -
CN              IF THE "HIGHER ENERGY BROAD GROUP NUMBER" IS NOT        -
CN              PROVIDED (COLS. 49-54 ARE BLANK OR ZERO), THE           -
CN              CONSTANTS SPECIFIED IN COLS. 13-48 WILL APPLY TO ALL    -
CN              BROAD GROUPS FOR THE PARTICULAR SCHEME.                 -
CN                                                                      -
CN              IF THE "LOWER ENERGY BROAD GROUP NUMBER" IS NOT         -
CN              PROVIDED (COLS. 55-60 ARE BLANK OR ZERO), THE           -
CN              CONSTANTS SPECIFIED IN COLS. 13-48 WILL APPLY TO THE    -
CN              HIGHER ENERGY BROAD GROUP NUMBER (COLS. 49-54) ONLY.    -
CN                                                                      -
CN              THE CONSTANTS DEFINING A PARTICULAR SCHEME CAN BE       -
CN              OVERLAYED. THAT IS, FACTORS DEFINED ON LATER TYPE 35    -
CN              CARDS SUPERCEDE DATA FOR ENERGY RANGES PREVIOUSLY       -
CN              DEFINED.                                                -
CN                                                                      -
CN              DIRECTIONAL DIFFUSION COEFFICIENT FACTOR SCHEMES ARE    -
CN              ASSIGNED TO COMPOSITIONS ON TYPE 36 CARDS.              -
CN                                                                      -
CN              IF NO TYPE 36 CARDS ARE SUPPLIED, AND ONLY ONE SCHEME   -
CN              IS DEFINED (THE SAME LABEL APPEARS IN COLS. 7-12 OF     -
CN              ALL TYPE 35 CARDS), THE FACTORS WILL BE USED IN ALL     -
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CN              COMPOSITIONS.
CN
CN              IF NO TYPE 36 CARDS ARE SUPPLIED AND MORE THAN ONE
CN              SCHEME IS DEFINED, THE FACTORS FOR THE FIRST DEFINED
CN              SCHEME (I.E. THAT SCHEME LABEL WHICH APPEARS ON THE
CN              FIRST TYPE 35 CARD) WILL BE USED IN ALL COMPOSITIONS.
CN
CN              THE CALCULATION OF TRANSVERSE LEAKAGE BY THE DIF3D
CN              CODE WILL USE THE THIRD DIMENSION DIFFUSION
CN              COEFFICIENT FOR THE PSEUDO ABSORPTION,
CN                    D-B-SQUARED = (A3*D+B3)*B**2
CN              REGARDLESS OF THE PROBLEM DIMENSIONS.  OTHER
CN              CODES USING THE COMPXS FILE MAY BEHAVE DIFFERENTLY -
CN              IT IS UP TO THE USER TO CHOOSE THE PROPER
CN              COEFFICIENT TO MODIFY.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          DIRECTIONAL DIFFUSION COEFFICIENT FACTORS-COMPOSITION
CR          CORRESPONDENCE (TYPE 36)
C
CL    FORMAT-----(I2,4X,11A6)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======  ==========================================================
CD    1-2      36
CD
CD    7-12     DIRECTIONAL DIFFUSION COEFFICIENT FACTOR SCHEME LABEL
CD             (SEE CARD TYPE 35).
CD
CD    13-18    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    19-24    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    25-30    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    31-36    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    37-42    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    43-48    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    49-54    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    55-60    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    61-66    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
CD
CD    67-72    COMPOSITION TO WHICH DIFFUSION COEFFICIENT FACTORS ARE
CD             ASSIGNED.
C
CN              IF MORE THAN ONE TYPE 36 CARD IS REQUIRED TO ASSIGN
CN              GIVEN DIFFUSION COEFFICIENT FACTORS TO COMPOSITIONS,
CN              THE LABEL IN COLS. 7-12 MUST BE REPEATED ON THE
CN              ADDITIONAL CARDS.
CN
CN              IF NO TYPE 36 CARDS ARE SUPPLIED, AND ONLY ONE
CN              DIRECTIONAL DIFFUSION COEFFICIENT FACTOR SCHEME IS
CN              DEFINED (THE SAME LABEL APPEARS IN COLS. 7-12 OF ALL
CN              TYPE 35 CARDS), THE FACTORS WILL BE USED IN ALL
CN              COMPOSITIONS.
CN
CN              IF NO TYPE 36 CARDS ARE SUPPLIED AND MORE THAN ONE
CN              SCHEME IS DEFINED, THE FACTORS FOR THE FIRST DEFINED
CN              SCHEME WILL BE USED IN ALL COMPOSITIONS.
CN
CN              IF NO COMPOSITIONS ARE DEFINED IN COLS. 13-72, THE
CN              SCHEME IDENTIFIED BY THE LABEL IN COLS. 7-12 WILL BE
CN              USED FOR ALL COMPOSITIONS.
CN
CN              THE SCHEME-COMPOSITION CORRESPONDENCE DATA CAN BE
CN              OVERLAYED. THAT IS, DATA GIVEN ON LATER TYPE 36 CARDS
CN              SUPERCEDES DATA PREVIOUSLY DEFINED.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          FISSION ENERGY CONVERSION FACTOR DATA (TYPE 37)
C
CL    FORMAT-----(I2,10X,3(A6,E12.5))
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======  ==========================================================
CD    1-2      37
CD
CD    13-18    COMPOSITION LABEL.
CD
CD    19-30    ENERGY CONVERSION FACTOR FOR THIS COMPOSITION
CD             (FISSIONS/WATT-SEC.).
CD
CD    31-36    COMPOSITION LABEL.
CD
CD    37-48    ENERGY CONVERSION FACTOR FOR THIS COMPOSITION
CD             (FISSIONS/WATT-SEC.).
CD
CD    49-54    COMPOSITION LABEL.
```

```
CD
CD    55-66     ENERGY CONVERSION FACTOR FOR THIS COMPOSITION
CD              (FISSIONS/WATT-SEC.).
C
CN              IF TYPE 37 OR TYPE 38 CARDS ARE PROVIDED FOR A
CN              A PARTICULAR COMPOSITION, THE ENERGY CONVERSION
CN              FACTORS IN DATA SET ISOTXS WILL BE IGNORED FOR THAT
CN              COMPOSITION, AND THE DATA ON THE TYPE 37 AND TYPE 38
CN              CARDS WILL BE USED INSTEAD.
CN
CN              IF THE FIRST LABEL (COLS. 13-18) ON A TYPE 37 CARD IS
CN              BLANK, THE ASSOCIATED CONVERSION FACTOR WILL BE
CN              ENTERED FOR ALL COMPOSITIONS.
CN
CN              IF COLS. 31-36 ARE BLANK THE DATA IN COLS. 37-66 ARE
CN              NEGLECTED.  IF COLS. 49-54 ARE BLANK THE DATA IN
CN              COLS. 55-66 ARE NEGLECTED.
CN
CN              DATA ON THIS CARD MAY BE OVERLAYED. THAT IS, FACTORS
CN              DEFINED ON LATER TYPE 37 CARDS SUPERCEDE DATA FOR
CN              COMPOSITIONS PREVIOUSLY SPECIFIED.
CN
CN              THE ENERGY CONVERSION FACTOR FOR ANY COMPOSITION NOT
CN              REFERENCED ON A TYPE 37 OR TYPE 38 CARD WILL BE
CN              DETERMINED FROM DATA IN ISOTXS.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          CAPTURE ENERGY CONVERSION FACTOR DATA (TYPE 38)
C
CL    FORMAT------(I2,10X,3(A6,E12.5))
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==========================================================
CD    1-2       38
CD
CD    13-18     COMPOSITION LABEL.
CD
CD    19-30     ENERGY CONVERSION FACTOR FOR THIS COMPOSITION
CD              (CAPTURES/WATT-SEC.).
CD
CD    31-36     COMPOSITION LABEL.
CD
CD    37-48     ENERGY CONVERSION FACTOR FOR THIS COMPOSITION
CD              (CAPTURES/WATT-SEC.).
CD
CD    49-54     COMPOSITION LABEL.
CD
CD    55-66     ENERGY CONVERSION FACTOR FOR THIS COMPOSITION
CD              (CAPTURES/WATT-SEC.).
C
CN              IF TYPE 37 OR TYPE 38 CARDS ARE PROVIDED FOR A
CN              A PARTICULAR COMPOSITION, THE ENERGY CONVERSION
CN              FACTORS IN DATA SET ISOTXS WILL BE IGNORED FOR THAT
CN              COMPOSITION, AND THE DATA ON THE TYPE 37 AND TYPE 38
CN              CARDS WILL BE USED INSTEAD.
CN
CN              IF THE FIRST LABEL (COLS. 13-18) ON A TYPE 38 CARD IS
CN              BLANK, THE ASSOCIATED CONVERSION FACTOR WILL BE
CN              ENTERED FOR ALL COMPOSITIONS.
CN
CN              IF COLS. 31-36 ARE BLANK THE DATA IN COLS. 37-66 ARE
CN              NEGLECTED.  IF COLS. 49-54 ARE BLANK THE DATA IN
CN              COLS. 55-66 ARE NEGLECTED.
CN
CN              DATA ON THIS CARD MAY BE OVERLAYED. THAT IS, FACTORS
CN              DEFINED ON LATER TYPE 38 CARDS SUPERCEDE DATA FOR
CN              COMPOSITIONS PREVIOUSLY SPECIFIED.
CN
CN              THE ENERGY CONVERSION FACTOR FOR ANY COMPOSITION NOT
CN              REFERENCED ON A TYPE 37 OR TYPE 38 CARD WILL BE
CN              DETERMINED FROM DATA IN ISOTXS.
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          NUCLIDE SET ASSIGNMENTS (TYPE 39)
C
CL    FORMAT------(I2,4X,11A6)
C
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY
CD    =======   ==========================================================
CD    1-2       39
CD
CD    7-12      NUCLIDE SET LABEL.
CD
CD    13-18     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    19-24     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    25-30     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    31-36     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    37-42     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    43-48     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    49-54     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    55-60     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    61-66     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
CD
CD    67-72     ISOTOPE TO BE ASSIGNED TO THIS NUCLIDE SET.
```

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C                                                                       -
CN              NUCLIDE SET ASSIGNMENTS ARE OPTIONAL. THEIR USE MAY     -
CN              REDUCE THE SIZE OF THE CCCC ATOM DENSITY FILE (ZNATDN)  -
CN              AND, THEREFORE, THE RUNNING TIME FOR CROSS SECTION      -
CN              HOMOGENIZATION.                                         -
CN                                                                      -
CN              ALL ISOTOPES USED IN A PARTICULAR ZONE OR A             -
CN              PARTICULAR SUBZONE MUST BE ASSIGNED TO THE SAME         -
CN              NUCLIDE SET.                                            -
CN                                                                      -
CN              WHEN NO TYPE 39 CARDS ARE PROVIDED, ALL ISOTOPES ARE    -
CN              ASSIGNED TO A SINGLE NUCLIDE SET.                       -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SOURCE EDIT AND SYNTHESIS TRIAL FUNCTION SOURCE             -
CR          SPECIFICATION (TYPE 40)                                     -
C                                                                       -
CL    FORMAT-----(I2,4X,4I6)                                            -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      40                                                       -
CD                                                                      -
CD    7-12     EDIT FLAG FOR POINTWISE INHOMOGENEOUS SOURCE             -
CD                 0, NO EDITS (DEFAULT).                               -
CD                 1, PRINT EDITS.                                      -
CD                 2, WRITE EDITS TO AUXILIARY OUTPUT FILE.             -
CD                 3, WRITE EDITS TO BOTH PRINT AND AUXILIARY OUTPUT    -
CD                    FILE.                                             -
CD                                                                      -
CD    13-18    RTFLUX FILE VERSION NUMBER FOR A SYNTHESIS TRIAL         -
CD             FUNCTION SOURCE.                                         -
CD                   S(X,Y,Z,G)=D(X,Y,Z,G)*FLUX(X,Y,Z,G)               -
CD             WHERE D IS A DIFFUSION COFFFICIENT AND FLUX IS A FLUX    -
CD             (OR ADJOINT FLUX) FROM AN INPUT RTFLUX (OR ATFLUX)       -
CD             FILE.  USE A NEGATIVE VALUE FOR ATFLUX.  SET TO ZERO     -
CD             WHEN ANOTHER TYPE OF SOURCE IS REQUIRED.                 -
CD                                                                      -
CD    19-24    VERSION NUMBER OF GEODST FILE SPECIFYING COMPOSITION     -
CD             DISTRIBUTION REQUIRED FOR A SYNTHESIS TRIAL FUNCTION     -
CD             SOURCE.  0 OR 1 IMPLIES THE GEOMETRY DEFINED BY THE      -
CD             CURRENT A.NIP3 DATASET.  THIS PARAMETER IS USED ONLY     -
CD             WHEN THE FLUX FILE VERSION IN COLS. 13-18 IS .GE. 1.     -
CD                                                                      -
CD    25-30    WORD LENGTH PARAMETER FOR THE FIXSRC FILE SOURCE         -
CD             DISTRIBUTION.  ON SINGLE-WORD-LENGTH MACHINES            -
CD             (E.G. CDC) THIS INPUT FIELD IS IGNORED.  ON DOUBLE-      -
CD             WORD-LENGTH MACHINES A VALUE OF 1 WILL PRODUCE A         -
CD             SHORT-WORD (I.E. REAL*4) FILE, A VALUE OF 2 WILL         -
CD             PRODUCE A DOUBLE-WORD (I.E. REAL*8) FILE.  THE DIF3D     -
CD             CODE REQUIRES A DOUBLE-WORD FILE  ON DOUBLE-WORD-        -
CD             LENGTH MACHINES.  (DEFAULT = 2 ON DOUBLE-WORD-LENGTH     -
CD             MACHINES)                                                -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          NATURAL DECAY INHOMOGENEOUS SOURCE SPECIFICATIONS           -
CR          (TYPE 41)                                                   -
C                                                                       -
CL    FORMAT-----(I2,4X,2(A6,E12.5,A6))                                 -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
CD    1-2      41                                                       -
C                                                                       -
CD    7-12     ISOTOPE LABEL                                            -
CD                                                                      -
CD    13-24    DECAY CONSTANT                                           -
CD                                                                      -
CD    25-30    SPECTRUM LABEL OF SPECTRUM TO BE USED WITH THIS          -
CD             ISOTOPE (SEE CARD TYPE 42)                               -
CD                                                                      -
CD    31-36    ISOTOPE LABEL                                            -
CD                                                                      -
CD    37-48    DECAY CONSTANT                                           -
CD                                                                      -
CD    49-54    SPECTRUM LABEL OF SPECTRUM TO BE USED WITH THIS          -
CD             ISOTOPE (SEE CARD TYPE 42)                               -
C                                                                       -
CN             WHEN THERE ARE TYPE 41 CARDS A FIXSRC FILE WILL BE       -
CN             CREATED CONTAINING THE DISTRIBUTED SOURCE                -
CN                     S(X,Y,Z,G) = SUM OVER ISOTOPES (I) OF            -
CN                       SCHI(G,I)*DC(I)*ATND(X,Y,Z,I)                  -
CN             WHERE SCHI IS AN ISOTOPE SOURCE SPECTRUM (SEE THE TYPE   -
CN             42 CARDS), DC IS THE DECAY CONSTANT AND ATND IS THE      -
CN             ISOTOPE NUMBER DENSITY.                                  -
CN                                                                      -
CN             AS MANY TYPE 41 CARDS SHOULD BE PROVIDED AS ARE          -
CN             NECESSARY TO SPECIFY ALL ISOTOPES REQUIRED.              -
CN                                                                      -
CN             WHEN THE SPECTRUM LABEL IS BLANK THE SOURCE WILL BE      -
CN             COMPUTED WITH THE SPECTRUM EQUAL TO 1.0 IN ALL GROUPS.   -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SOURCE SPECTRUM DATA (TYPE 42)                              -
C                                                                       -
CL    FORMAT-----(I2,4X,A6,5E12.5)                                      -
C                                                                       -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                  -
CD    =======  ========================================================-
```

```
CD    1-2       42                                                          -
CD                                                                          -
CD    7-12      SPECTRUM LABEL                                              -
CD                                                                          -
CD    13-24     GROUP MULTIPLIER (SPECTRUM), FIRST GROUP.                   -
CD                                                                          -
CD    25-36     GROUP MULTIPLIER (SPECTRUM), NEXT GROUP.                    -
CD                                                                          -
CD    37-48     GROUP MULTIPLIER (SPECTRUM), NEXT GROUP.                    -
CD                                                                          -
CD    49-60     GROUP MULTIPLIER (SPECTRUM), NEXT GROUP.                    -
CD                                                                          -
CD    61-72     GROUP MULTIPLIER (SPECTRUM), NEXT GROUP.                    -
C                                                                           -
CN              AS MANY TYPE 42 CARDS, FIVE ENERGY GROUPS PER CARD,         -
CN              SHOULD BE PROVIDED AS ARE NECESSARY TO SPECIFY ALL THE      -
CN              SPECTRA NEEDED FOR THE NATURAL DECAY SOURCE                 -
CN              CALCULATION.  THE FIRST TYPE 42 CARD MUST HAVE A            -
CN              NON-BLANK SPECTRUM LABEL.  A REPEATED SPECTRUM LABEL        -
CN              IMPLIES A CONTINUATION OF THE LAST CARD WITH THE SAME       -
CN              LABEL.  A BLANK SPECTRUM LABEL IMPLIES A CONTINUATION       -
CN              OF THE SPECTRUM ON THE PREVIOUS TYPE 42 CARD.               -
CN                                                                          -
CN              WHEN THE NUMBER OF DATA FOR A PARTICULAR SPECTRUM IS        -
CN              LESS THAN THE TOTAL NUMBER OF ENERGY GROUPS, THE            -
CN              REMAINING ELEMENTS OF THE SPECTRUM ARE SET TO ZERO.         -
CN              WHEN THE NUMBER OF DATA IS GREATER THAN THE NUMBER          -
CN              OF GROUPS THE SURPLUS ELEMENTS ARE IGNORED.                 -
C                                                                           -
C-------------------------------------------------------------------------
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```
C-------------------------------------------------------------------------
CR          GRAPHICS OUTPUT CONTROL (TYPE 43)                               -
C                                                                           -
CL    FORMAT-----(I2,4X,I6,3E12.4,3I6)                                      -
C                                                                           -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                      -
CD    =======  ========================================================     -
CD    1-2      43                                                           -
CD                                                                          -
CD    7-12     GRAPHICS OUTPUT SENTINEL FOR MAP                             -
CD             0...NO GRAPHICS (DEFAULT)                                    -
CD             1...GENERATE MAP                                             -
CD                                                                          -
CD    13-24    HEIGHT OF GRAPHICS OUTPUT FIELD (DEFAULT=11.0 INCHES)        -
CD                                                                          -
CD    25-36    WIDTH OF GRAPHICS OUTPUT FIELD (DEFAULT=11.0 INCHES)         -
CD                                                                          -
CD    37-48    FOR TRIANGULAR AND HEXAGONAL GEOMETRIES - THIS FIELD         -
CD             CONTAINS THE FLAT-TO-FLAT DISTANCE ACROSS EACH               -
CD             HEXAGON, IN INCHES (DEFAULT = 0.5 INCHES)                    -
CD                                                                          -
CD             FOR ORTHOGONAL GEOMETRIES - THIS FIELD CONTAINS THE          -
CD             MINIMUM REDUCTION ALLOWED FOR LABELS (DEFAULT = 0.5).        -
CD             SEE THE NOTE BELOW.                                          -
C                                                                           -
CD    49-54    PRINTER PLOTTER SENTINEL - HEXAGONAL MAP ONLY                -
CD             1...FLAT-TO-FLAT HEXAGON DIMENSION = 8 ROWS                  -
CD             2...FLAT-TO-FLAT HEXAGON DIMENSION = 6 ROWS (DEFAULT)        -
CD                                                                          -
CD    55-60    MAXIMUM NO. OF ROWS IN PRINTER-PLOTTER FIELD -               -
CD             HEXAGONAL MAP ONLY (DEFAULT = 48)                            -
CD                                                                          -
CD    61-66    MAXIMUM NO. OF PRINT COLUMNS IN PRINTER-PLOTTER FIELD        -
CD             - HEXAGONAL MAP ONLY (DEFAULT = 130)                         -
C                                                                           -
CN              THE GRAPHICS OPTION MAY NOT BE AVAILABLE IN ALL              -
CN              VERSIONS OF THE INPUT PROCESSOR GNIP4C.                      -
CN                                                                          -
CN              THIS CARD CONTROLS THE FORMAT OF THE PRINTER-PLOTTER         -
CN              OUTPUT FOR HEXAGONAL MAPS BUT DOES NOT ACTUALLY              -
CN              TRIGGER THE PRINTER MAP.  THAT IS DONE BY A SENTINEL         -
CN              ON THE TYPE 02 CARD.  THIS CARD HAS NO EFFECT ON THE         -
CN              PRINTER-PLOTTER MAP OF ORTHOGONAL GEOMETRY MODELS.           -
CN                                                                          -
CN              FOR TRIANGULAR AND HEXAGONAL GEOMETRIES THE SCALE            -
CN              OF THE PLOT IS DETERMINED BY THE FLAT-TO-FLAT DISTANCE       -
CN              IN COLS. 37-48.  THE SIZE OF THE GRAPHICS PAGE IS SET        -
CN              BY THE DATA IN COLS. 13-36.  THE CODE GENERATES AS           -
CN              MANY PAGES OF GRAPHICS OUTPUT AS IT TAKES TO COVER THE       -
CN              ENTIRE MAP.  LABELS ARE CENTERED IN EACH HEXAGON, AND        -
CN              THE CHARACTER SIZE IS A FIXED FRACTION (1/8) OF THE          -
CN              FLAT-TO-FLAT DISTANCE.                                       -
CN                                                                          -
CN              FOR ORTHOGONAL GEOMETRIES THE SCALE OF THE PLOT IS           -
CN              SET BY THE CODE SO THAT THE ENTIRE MAP IS FORCED             -
CN              TO FIT IN A SINGLE GRAPHICS PAGE.  THE MAXIMUM               -
CN              SIZE OF THE GRAPHICS PAGE IS SET BY THE DATA IN              -
CN              COLS. 13-36.  LABELS WITH 0.1 INCH CHARACTER HEIGHT          -
CN              ARE PLACE IN REGIONS AS LONG AS THERE IS ROOM.  IF THE       -
CN              REGION IS TOO SMALL, THE LABEL IS REDUCED IN SIZE.  IF       -
CN              TO FIT IN THE REGION THE LABEL SIZE MUST BE REDUCED          -
CN              BY A FACTOR SMALLER THAN THE NUMBER IN COLS. 37-48           -
CN              NO LABEL IS DRAWN.  WHEN THE NUMBER IN COLS. 37-48           -
CN              IS GREATER THAN 1.0 NO LABELS ARE DRAWN.                     -
C                                                                           -
C-------------------------------------------------------------------------
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C-------------------------------------------------------------------------
CR        ASSIGNMENT OF REGIONS TO CONTROL ROD BANKS (TYPE 44)              -
C                                                                           -
CL    FORMAT-----(I2,4X,11A6)                                               -
C                                                                           -
CD    COLUMNS          CONTENTS...IMPLICATIONS, IF ANY                      -
CD    =======  ========================================================     -
CD    1-2      44                                                           -
CD                                                                          -
```

```
CD     7-12      CONTROL ROD BANK LABEL (REPEATED ON ADDITIONAL          -
CD               TYPE 44 CARDS IF NECESSARY).                            -
CD                                                                       -
CD     13-18     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     19-24     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     25-30     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     31-36     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     37-42     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     43-48     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     49-54     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     55-60     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     61-66     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
CD                                                                       -
CD     67-72     REGION LABEL OR AREA LABEL DEFINING REGION(S)           -
CD               AT THE TIP OF THE MOVEABLE PORTION OF THE ROD(S) IN     -
CD               THE SPECIFIED CONTROL ROD BANK.                         -
C                                                                        -
CN               ALL REGIONS IN A ROD CHANNEL ABOVE THE ROD TIP          -
CN               MOVE TOGETHER.  ALL REGIONS BELOW THE TIP ARE           -
CN               STATIONARY, AND ARE REPLACED BY ROD REGIONS AS THE      -
CN               ROD MOVES DOWN.  THE TOPMOST REGION IN THE ROD          -
CN               EXPANDS AS THE ROD MOVES DOWN FROM ITS INITIAL          -
CN               POSITION.  THE REGION JUST BELOW THE INITIAL ROD-TIP    -
CN               POSITION EXPANDS AS THE ROD MOVES UP FROM ITS           -
CN               ORIGINAL POSITION.                                      -
CN                                                                       -
CN               THE LOWER BOUNDARY OF ALL ROD-TIP REGIONS WHICH DEFINE  -
CN               ROWS ASSIGNED TO A PARTICULAR CONTROL ROD BANK MUST     -
CN               BE AT THE SAME AXIAL POSITION.  "AXIAL" REFERS TO THE   -
CN               Z-DIMENSION IN RZ, XYZ, AND HEX-Z, AND TO THE Y         -
CN               DIMENSION IN XY.  THUS FOR THE (R-Z E.G.) GEOMETRY      -
CN               PICTURED BELOW,                                         -
CN                                                                       -
CN               ---------------------------------------                 -
CN               |       |       |       |       |       |             -
CN               |       |  R2   |       |  R6   | CR21  |             -
CN               |       |       |       |       |       |             -
CN               |       |-------|  CR11 |-------|-------|             -
CN               |       |       |       |       |       |             -
CN               |       |  R3   |       |       |  CR22 |             -
CN               |       |       |       |       |       |             -
CN               |  R1   |-------|-------|  R7   |-------|             -
CN               |       |       |       |       |       |             -
CN               |       |  R4   |  CR12 |       |  CR23 |             -
CN               |       |       |       |       |       |             -
CN               |       |-------|-------|-------|-------|             -
CN               |       |       |       |       |       |             -
CN               |       |  R5   |  C1   |  R8   |  C2   |             -
CN               |       |       |       |       |       |             -
CN               ---------------------------------------                 -
CN                                                                       -
CN               THE FOLLOWING TYPE 44 CARDS (GIVEN IN FREE FORMAT       -
CN               STYLE INPUT) WOULD RESULT IN A FATAL ERROR              -
CN                                                                       -
CN                     44 BANK1 CR12 CR22                                -
CN                                                                       -
CN               WHEREAS                                                 -
CN                                                                       -
CN                     44 BANK1 CR12 CR23                                -
CN                                                                       -
CN               WOULD BE ACCEPTABLE.  ALSO, A ROD BANK MAY NOT BE       -
CN               SPECIFIED USING MORE THAN ONE REGION IN A PARTICULAR    -
CN               VERTICAL CHANNEL.  THUS                                 -
CN                                                                       -
CN                     44 BANK1 CR22 CR23                                -
CN                                                                       -
CN               WOULD LEAD TO A FATAL INPUT ERROR.                      -
CN                                                                       -
CN               NOTE THAT SINCE IT MUST BE ASSUMED THAT A CONTROL ROD   -
CN               BANK WILL BE MOVED DURING THE COURSE OF A PROBLEM,      -
CN               AT LEAST ONE REGION MUST BE DEFINED BELOW EACH REGION   -
CN               SPECIFIED IN COLS. 13-72.  THUS, THE FOLLOWING TYPE     -
CN               44 CARD WOULD NOT BE ACCEPTABLE FOR THE GEOMETRY GIVEN  -
CN               ABOVE                                                   -
CN                     44 BANK1 C1                                       -
CN                                                                       -
CN               AN AREA LABEL IN COLS. 13-72 IMPLIES ALL THE REGIONS    -
CN               ASSIGNED TO THAT AREA.  AREAS ARE DEFINED ON THE        -
CN               TYPE 07 CARD OF DATASET A.NIP3.                         -
CN                                                                       -
CN               THE FIRST BLANK REGION LABEL ENCOUNTERED TERMINATES     -
CN               READING OF THE DATA ON THAT PARTICULAR TYPE 44 CARD.    -
CN                                                                       -
CN               NOTE THAT A BLANK CONTROL ROD BANK LABEL IS ACCEPTABLE. -
C                                                                        -
C-------------------------------------------------------------------------

CEOF
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Appendix C

DIF3D CCCC BINARY INTERFACE FILE DESCRIPTIONS

C.1 ISOTXS

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C*****************************************************************************
C                       REVISED 11/30/76                                      -
C                                                                             -
CF          ISOTXS-IV                                                         -
CE          MICROSCOPIC GROUP NEUTRON CROSS SECTIONS                          -
C                                                                             -
CN                      THIS FILE PROVIDES A BASIC BROAD GROUP                -
CN                      LIBRARY, ORDERED BY ISOTOPE                           -
CN                      FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES          -
CN                      ONLY.                                                 -
C                                                                             -
C*****************************************************************************
C-----------------------------------------------------------------------------
CS          FILE STRUCTURE                                                    -
CS                                                                            -
CS             RECORD TYPE                          PRESENT IF                -
CS             ===========                          ==========                -
CS             FILE IDENTIFICATION                  ALWAYS                    -
CS             FILE CONTROL                         ALWAYS                    -
CS             FILE DATA                            ALWAYS                    -
CS             FILE-WIDE CHI DATA                   ICHIST.GT.1               -
CS                                                                            -
CS   **************(REPEAT FOR ALL ISOTOPES)                                 -
CS   *          ISOTOPE CONTROL AND GROUP                                    -
CS   *                        INDEPENDENT DATA     ALWAYS                    -
CS   *          PRINCIPAL CROSS SECTIONS           ALWAYS                    -
CS   *          ISOTOPE CHI DATA                   ICHI.GT.1                 -
CS   *                                                                       -
CS   *  ************(REPEAT TO NSCMAX SCATTERING BLOCKS)                     -
CS   *  *  ********(REPEAT FROM 1 TO NSBLOK)                                 -
CS   *  *  *    SCATTERING SUB-BLOCK             LORD(N).GT.0              -
CS   **************                                                          -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          FILE IDENTIFICATION                                               -
C                                                                             -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                             -
C                                                                             -
CW    1+3*MULT=NUMBER OF WORDS                                                -
C                                                                             -
CB     FORMAT(11H 0V ISOTXS ,   1H*,                                          -
CB    12A6,1H*,I6)                                                            -
C                                                                             -
CD     HNAME          HOLLERITH FILE NAME = ISOTXS = (A6)                     -
CD     HUSE(I)        HOLLERITH USER IDENTIFICATION (A6)                      -
CD     IVERS          FILE VERSION NUMBER                                     -
CD     MULT           DOUBLE PRECISION PARAMETER                              -
CD                        1= A6 WORD IS SINGLE WORD                            -
CD                        2= A6 WORD IS DOUBLE PRECISION WORD                  -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          FILE CONTROL   (1D RECORD)                                        -
C                                                                             -
CL    NGROUP,NISO,MAXUP,MAXDN,MAXORD,ICHIST,NSCMAX,NSBLOK                     -
C                                                                             -
CW    8=NUMBER OF WORDS                                                       -
C                                                                             -
CB    FORMAT(4H 1D ,8I6)                                                      -
C                                                                             -
CD    NGROUP         NUMBER OF ENERGY GROUPS IN FILE                         -
CD    NISO           NUMBER OF ISOTOPES IN FILE                              -
CD    MAXUP          MAXIMUM NUMBER OF UPSCATTER GROUPS                      -
CD    MAXDN          MAXIMUM NUMBER OF DOWNSCATTER GROUPS                    -
CD    MAXORD         MAXIMUM SCATTERING ORDER (MAXIMUM VALUE OF              -
CD                      LEGENDRE EXPANSION INDEX USED IN FILE).               -
CD    ICHIST         FILE-WIDE FISSION SPECTRUM FLAG                         -
CD                      ICHIST.EQ.0,       NO FILE-WIDE SPECTRUM             -
CD                      ICHIST.EQ.1,       FILE-WIDE CHI VECTOR              -
CD                      ICHIST.GT.1,       FILE-WIDE CHI MATRIX              -
CD    NSCMAX         MAXIMUM NUMBER OF BLOCKS OF SCATTERING DATA             -
CD    NSBLOK         SUBBLOCKING CONTROL FOR SCATTER MATRICES. THE           -
CD                      SCATTERING DATA ARE SUBBLOCKED INTO NSBLOK            -
CD                      RECORDS(SUBBLOCKS) PER SCATTERING BLOCK.              -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          FILE DATA   (2D RECORD)                                           -
C                                                                             -
CL    (HSETID(I),I=1,12),(HISONM(I),I=1,NISO),                                -
CL   1(CHI(J),J=1,NGROUP),(VEL(J),J=1,NGROUP),                                -
CL   2(EMAX(J),J=1,NGROUP),EMIN,(LOCA(I),I=1,NISO)                            -
C                                                                             -
CW    (NISO+12)*MULT+1+NISO                                                   -
CW    +NGROUP*(2+ICHIST*(2/(ICHIST+1)))=NUMBER OF WORDS                       -
C                                                                             -
CB    FORMAT(4H 2D ,1H*,11A6,1H*/      HSETID,HISONM                          -
CB   11H*,A6,1H*,9(1X,A6)/(10(1X,A6)))                                        -
CB    FORMAT(  6E12.5)                 CHI (PRESENT IF ICHIST.EQ.1)           -
CB    FORMAT ( 6E12.5)                 VEL,EMAX,EMIN                          -
CB    FORMAT(12I6)                     LOCA                                   -
C                                                                             -
CD    HSETID(I)      HOLLERITH IDENTIFICATION OF FILE (A6)                    -
CD    HISONM(I)      HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6)               -
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CD    CHI(J)        FILE-WIDE FISSION SPECTRUM(PRESENT IF ICHIST.EQ.1) -
CD    VEL(J)        MEAN NEUTRON VELOCITY IN GROUP J (CM/SEC)          -
CD    EMAX(J)       MAXIMUM ENERGY BOUND OF GROUP J (EV)               -
CD    EMIN          MINIMUM ENERGY BOUND OF SET (EV)                   -
CD    LOCA(I)       NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR   -
CD                     ISOTOPE I.  LOCA(1)=0                           -
C                                                                       -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          FILE-WIDE CHI DATA   (3D RECORD)                            -
C                                                                       -
CC        PRESENT IF ICHIST.GT.1                                        -
C                                                                       -
CL    ((CHI(K,J),K=1,ICHIST),J=1,NGROUP),(ISSPEC(I),I=1,NGROUP)         -
C                                                                       -
CW    NGROUP*(ICHIST+1)=NUMBER OF WORDS                                 -
C                                                                       -
CB    FORMAT(4H 3D ,  5E12.5/(6E12.5)) CHI                              -
CB    FORMAT(12I6)                     ISSPEC                           -
C                                                                       -
CD    CHI(K,J)      FRACTION OF NEUTRONS EMITTED INTO GROUP J AS A      -
CD                     RESULT OF FISSION IN ANY GROUP,USING SPECTRUM K  -
CD    ISSPEC(I)     ISSPEC(I)=K IMPLIES THAT SPECTRUM K IS USED         -
CD                     TO CALCULATE EMISSION SPECTRUM FROM FISSION      -
CD                     IN GROUP I                                       -
C                                                                       -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          ISOTOPE CONTROL AND GROUP INDEPENDENT DATA   (4D RECORD)    -
C                                                                       -
CL    HABSID,HIDENT,HMAT,AMASS,EFISS,ECAPT,TEMP,SIGPOT,ADENS,KBR,ICHI,  -
CL   1IFIS,IALF,INP,IN2N,IND,INT,LTOT,LTRN,ISTRPD,                      -
CL   2(IDSCT(N),N=1,NSCMAX),(LORD(N),N=1,NSCMAX),                       -
CL   3((JBAND(J,N),J=1,NGROUP),N=1,NSCMAX),                             -
CL   4((IJJ(J,N),J=1,NGROUP),N=1,NSCMAX)                                -
C                                                                       -
CW    3*MULT+17+NSCMAX*(2*NGROUP+2)=NUMBER OF WORDS                     -
C                                                                       -
CB    FORMAT(4H 4D ,3(1X,A6)/  6E12.5/                                  -
CB   1(12I6))                                                           -
C                                                                       -
CD    HABSID        HOLLERITH ABSOLUTE ISOTOPE LABEL - SAME FOR ALL     -
CD                        VERSIONS OF THE SAME ISOTOPE IN FILE (A6)     -
CD    HIDENT        IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA         -
CD                        CAME(E.G. ENDF/B) (A6)                        -
CD    HMAT          ISOTOPE IDENTIFICATION (E.G. ENDF/B MAT NO.) (A6)   -
CD    AMASS         GRAM ATOMIC WEIGHT                                  -
CD    EFISS         TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)     -
CD    ECAPT         TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/CAPT)     -
CD    TEMP          ISOTOPE TEMPERATURE (DEGREES KELVIN)                -
CD    SIGPOT        AVERAGE EFFECTIVE POTENTIAL SCATTERING IN           -
CD                        RESONANCE RANGE (BARNS/ATOM)                  -
CD    ADENS         DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE      -
CD                        CROSS SECTIONS WERE GENERATED (A/BARN-CM)-
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CD    KBR           ISOTOPE CLASSIFICATION                              -
CD                     0=UNDEFINED                                      -
CD                     1=FISSILE                                        -
CD                     2=FERTILE                                        -
CD                     3=OTHER ACTINIDE                                 -
CD                     4=FISSION PRODUCT                                -
CD                     5=STRUCTURE                                      -
CD                     6=COOLANT                                        -
CD                     7=CONTROL                                        -
CD    ICHI          ISOTOPE FISSION SPECTRUM FLAG                       -
CD                      ICHI.EQ.0,     USE FILE-WIDE CHI                -
CD                      ICHI.EQ.1,     ISOTOPE CHI VECTOR               -
CD                      ICHI.GT.1,     ISOTOPE CHI MATRIX               -
CD    IFIS          (N,F) CROSS SECTION FLAG                            -
CD                     IFIS=0, NO FISSION DATA IN PRINCIPAL CROSS        -
CD                                  SECTION RECORD                       -
CD                        =1, FISSION DATA PRESENT IN PRINCIPAL          -
CD                                  CROSS SECTION RECORD                 -
CD    IALF          (N,ALPHA) CROSS SECTION FLAG                        -
CD                     SAME OPTIONS AS IFIS                             -
CD    INP           (N,P) CROSS SECTION FLAG                            -
CD                     SAME OPTIONS AS IFIS                             -
CD    IN2N          (N,2N) CROSS SECTION FLAG                           -
CD                     SAME OPTIONS AS IFIS                             -
CD    IND           (N,D) CROSS SECTION FLAG                            -
CD                     SAME OPTIONS AS IFIS                             -
CD    INT           (N,T) CROSS SECTION FLAG                            -
CD                     SAME OPTIONS AS IFIS                             -
CD    LTOT          NUMBER OF MOMENTS OF TOTAL CROSS SECTION PROVIDED   -
CD                     IN PRINCIPAL CROSS SECTIONS RECORD               -
CD    LTRN          NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION        -
CD                     PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD      -
CD    ISTRPD        NUMBER OF COORDINATE DIRECTIONS FOR WHICH           -
CD                     COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS    -
CD                     ARE GIVEN. IF ISTRPD=0, NO COORDINATE DEPENDENT  -
CD                     TRANSPORT CROSS SECTIONS ARE GIVEN.              -
CD    IDSCT(N)      SCATTERING MATRIX TYPE IDENTIFICATION FOR           -
CD                     SCATTERING BLOCK N.  SIGNIFICANT ONLY IF         -
CD                     LORD(N).GT.0                                     -
CD                     IDSCT(N)=000 + NN, TOTAL SCATTERING, (SUM OF     -
CD                         ELASTIC,INELASTIC, AND N,2N SCATTERING       -
CD                         MATRIX TERMS).                               -
CD                             =100 + NN, ELASTIC SCATTERING            -
CD                             =200 + NN, INELASTIC SCATTERING          -
CD                             =300 + NN, (N,2N) SCATTERING,----SEE     -
CD                              NOTE BELOW----                          -
CD                     WHERE NN IS THE LEGENDRE EXPANSION INDEX OF THE  -
CD                     FIRST MATRIX IN BLOCK N                          -
CD    LORD(N)       NUMBER OF SCATTERING ORDERS IN BLOCK N.  IF         -
CD                     LORD(N)=0, THIS BLOCK IS NOT PRESENT FOR THIS    -
CD                     ISOTOPE.  IF NN IS THE VALUE TAKEN FROM          -
CD                     IDSCT(N), THEN THE MATRICES IN THIS BLOCK        -
CD                     HAVE LEGENDRE EXPANSION INDICES OF NN,NN+1,      -
CD                     NN+2,...,NN+LORD(N)-1                            -
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C     JBAND(J,N)    NUMBER OF GROUPS THAT SCATTER INTO GROUP J,
C                      INCLUDING SELF-SCATTER, IN SCATTERING BLOCK N.
C                      IF JBAND(J,N)=0, NO SCATTER DATA IS PRESENT IN
C                      BLOCK N
C     IJJ(J,N)      POSITION OF IN-GROUP SCATTERING CROSS SECTION IN
C                      SCATTERING DATA FOR GROUP J, SCATTERING BLOCK
C                      N,COUNTED FROM THE FIRST WORD OF GROUP J DATA.
C                      IF JBAND(J,N).NE.0 THEN IJJ(J,N) MUST SATISFY
C                      THE RELATION 1.LE.IJJ(J,N).LE.JBAND(J,N)
C
C                   NOTE- FOR N,2N SCATTER, THE MATRIX CONTAINS TERMS,
C                      SCAT(J TO G), WHICH ARE EMISSSION (PRODUCTION)-
C                      BASED, I.E., ARE DEFINED SUCH THAT MACROSCOPIC
C                      SCAT(J TO G) TIMES THE FLUX IN GROUP J GIVES
C                      THE RATE OF EMISSION (PRODUCTION) OF  NEUTRONS
C                      INTO GROUP G.
C
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          PRINCIPAL CROSS SECTIONS   (5D RECORD)
C
CL    ((STRPL(J,L),J=1,NGROUP),L=1,LTRN),
CL   1((STOTPL(J,L),J=1,NGROUP),L=1,LTOT),(SNGAM(J),J=1,NGROUP),
CL   2(SFIS(J),J=1,NGROUP),(SNUTOT(J),J=1,NGROUP),
CL   3(CHISO(J),J=1,NGROUP),(SNALF(J),J=1,NGROUP),
CL   4(SNP(J),J=1,NGROUP),(SN2N(J),J=1,NGROUP),
CL   5(SND(J),J=1,NGROUP),(SNT(J),J=1,NGROUP)
CL   6((STRPD(J,I),J=1,NGROUP),I=1,ISTRPD)
C
CW    (1+LTRN+LTOT+IALF+INP+IN2N+IND+INT+ISTRPD+2*IFIS+
CW    ICHI*(2/(ICHI+1)))*NGROUP=NUMBER OF WORDS
C
CB    FORMAT(4H 5D ,  5E12.5/(6E12.5)) LENGTH OF LIST AS ABOVE
C
C     STRPL(J,L)     PL WEIGHTED TRANSPORT CROSS SECTION
C                       THE FIRST ELEMENT OF ARRAY STRPL IS THE
C                       CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION
C                       THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1)
C                       IS NOT INCLUDED IN STRPL(J,L).
C     STOTPL(J,L)    PL WEIGHTED TOTAL CROSS SECTION
C                       THE FIRST ELEMENT OF ARRAY STOTPL IS THE
C                       FLUX (P0) WEIGHTED TOTAL CROSS SECTION
C                       THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1)
C                       IS NOT INCLUDED IN STOTPL(J,L).
C     SNGAM(J)       (N,GAMMA)
C     SFIS(J)        (N,F)          (PRESENT IF IFIS.GT.0)
C     SNUTOT(J)      TOTAL NEUTRON YIELD/FISSION  (PRESENT IF IFIS.GT.0)
C     CHISO(J)       ISOTOPE CHI  (PRESENT IF ICHI.EQ.1)
C     SNALF(J)       (N,ALPHA)    (PRESENT IF IALF.GT.0)
C     SNP(J)         (N,P)        (PRESENT IF INP.GT.0)
C     SN2N(J)        (N,2N)       (PRESENT IF IN2N.GT.0)  ----SEE
C                       NOTE BELOW----
C     SND(J)         (N,D)        (PRESENT IF IND.GT.0)
C     SNT(J)         (N,T)        (PRESENT IF INT.GT.0)
CD    STRPD(J,I)     COORDINATE DIRECTION I TRANSPORT CROSS SECTION
CD                      (PRESENT IF ISTRPD.GT.0)
C
CN                  NOTE - THE PRINCIPAL N,2N CROSS SECTION SN2N(J)
CN                     IS DEFINED AS THE N,2N REACTION CROSS SECTION,
CN                     I.E., SUCH THAT MACROSCOPIC SN2N(J) TIMES THE
CN                     FLUX IN GROUP J GIVES THE RATE AT WHICH N,2N
CN                     REACTIONS OCCUR IN GROUP J.  THUS, FOR N,2N
CN                     SCATTERING, SN2N(J) = 0.5*(SUM OF SCAT(J TO G)
CN                     SUMMED OVER ALL G).
C
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          ISOTOPE CHI DATA   (6D RECORD)
C
CC          PRESENT IF ICHI.GT.1
C
CL    ((CHIISO(K,J),K=1,ICHI),J=1,NGROUP),(ISOPEC(I),I=1,NGROUP)
C
CW    NGROUP*(ICHI+1)=NUMBER OF WORDS
C
CB    FORMAT(4H 6D ,  5E12.5/(6E12.5)) CHIISO
CB    FORMAT(12I6)                     ISOPEC
C
CD    CHIISO(K,J)    FRACTION OF NEUTRONS EMITTED INTO GROUP J AS A
CD                      RESULT OF FISSION IN ANY GROUP,USING SPECTRUM K
CD    ISOPEC(I)      ISOPEC(I)=K IMPLIES THAT SPECTRUM K IS USED
CD                      TO CALCULATE EMISSION SPECTRUM FROM FISSION
CD                      IN GROUP I
C
C
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          SCATTERING SUB-BLOCK   (7D RECORD)
C
CC        PRESENT IF LORD(N).GT.0
C
CL    ((SCAT(K,L),K=1,KMAX),L=1,LORDN)
C
CC    KMAX=SUM OVER J OF JBAND(J,N) WITHIN THE J-GROUP RANGE OF THIS
CC       SUB-BLOCK.  IF M IS THE INDEX OF THE SUB-BLOCK, THE J-GROUP
CC       RANGE CONTAINED WITHIN THIS SUB-BLOCK IS
CC       JL=(M-1)*((NGROUP-1)/NSBLOK+1)+1 TO JU=MIN0(NGROUP,JUP),
CC       WHERE JUP=M*((NGROUP-1)/NSBLOK +1).
C
CC    LORDN=LORD(N)
CC    N IS THE INDEX FOR THE LOOP OVER NSCMAX (SEE FILE STRUCTURE)
C
CW    KMAX*LORDN=NUMBER OF WORDS
C
CB    FORMAT(4H 7D ,  5E12.5/(6E12.5))
C
CD    SCAT(K,L)      SCATTERING MATRIX OF SCATTERING ORDER L, FOR
CD                      REACTION TYPE IDENTIFIED BY IDSCT(N) FOR THIS
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CD                    BLOCK.  JBAND(J,N) VALUES FOR SCATTERING INTO   -
CD                    GROUP J ARE STORED AT LOCATIONS K=SUM FROM 1    -
CD                    TO (J-1) OF JBAND(J,N) PLUS 1 TO K-1+JBAND(J,N).-
CD                    THE SUM IS ZERO WHEN J=1.  J-TO-J SCATTER IS    -
CD                    THE IJJ(J,N)-TH ENTRY IN THE RANGE JBAND(J,N).  -
CD                    VALUES ARE STORED IN THE ORDER (J+JUP),         -
CD                    (J+JUP-1),...,(J+1),J,(J-1),...,(J-JDN),        -
CD                    WHERE JUP=IJJ(J,N)-1 AND JDN=JBAND(J,N)-IJJ(J,N)-
C                                                                     -
C---------------------------------------------------------------------
CEOF
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C.2 GEODST

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C*********************************************************************
C                       REVISED 11/30/76                              -
C                                                                     -
CF          GEODST - IV                                               -
C                                                                     -
CE          GEOMETRY DESCRIPTION                                      -
C                                                                     -
C*********************************************************************
C---------------------------------------------------------------------
CR          FILE IDENTIFICATION (OV RECORD)                           -
C                                                                     -
CL     HNAME,(HUSE(I),I=1,2),IVERS                                    -
C                                                                     -
CW     1+3*MULT                                                       -
C                                                                     -
CD     HNAME              HOLLERITH FILE NAME - GEODST - (A6)         -
CD     HUSE               HOLLERITH USER IDENTIFICATION (A6)          -
CD     IVERS              FILE VERSION NUMBER                         -
CD     MULT               DOUBLE PRECISION PARAMETER                  -
CD                            1- A6 WORD IS SINGLE WORD               -
CD                            2- A6 WORD IS DOUBLE PRECISION WORD     -
C                                                                     -
C---------------------------------------------------------------------
C---------------------------------------------------------------------
CR          FILE SPECIFICATIONS (1D RECORD)                           -
C                                                                     -
CL     ICOM,NZONE,NREG,NZCL,NCINTI,NCINTJ,NCINTK,NINTI,NINTJ,NINTK,IMB1,-
CL     IMB2,JMB1,JMB2,KMB1,KMB2,NBS,NBCS,NIBCS,NZWBB,NTRIAG,NRASS,NTHPT,-
CL     (NGOP(I),I=1,4)                                                -
C                                                                     -
CW     27                                                             -
C                                                                     -
CD     ICOM               GEOMETRY  0- POINT (FUNDAMENTAL MODE)       -
CD                                   1- SLAB                          -
CD                                   2- CYLINDER                      -
CD                                   3- SPHERE                        -
CD                                   6- X-Y                           -
CD                                   7- R-Z                           -
CD                                   8- THETA-R                       -
CD                                   9- UNIFORM TRIANGULAR            -
CD                                  10- HEXAGONAL (1 MESH POINT IN EACH -
CD                                                HEXAGONAL ELEMENT)  -
CD                                  11- R-THETA                       -
CD                                  12- R-THETA-Z                     -
CD                                  13- R-THETA-ALPHA                 -
CD                                  14- X-Y-Z                         -
CD                                  15- THETA-R-Z                     -
CD                                  16- THETA-R-ALPHA                 -
CD                                  17- UNIFORM TRIANGULAR-Z          -
CD                                  18- HEXAGON-Z   (MESH POINTS AS IN 10 -
CD                                                   ABOVE)         -
CD     NZONE              NUMBER OF ZONES (EACH HOMOGENEOUS IN NEUTRONICS-
CD                        PROBLEM - A ZONE CONTAINS ONE OR MORE REGIONS) -
CD     NREG               NUMBER OF REGIONS                           -
CD     NZCL               NUMBER OF ZONE CLASSIFICATIONS (EDIT PURPOSES) -
CD     NCINTI             NUMBER OF FIRST DIMENSION COARSE MESH INTERVALS-
CD     NCINTJ             NUMBER OF SECOND DIMENSION COARSE MESH      -
CD                            INTERVALS. NCINTJ.EQ.1 FOR ONE DIMENSIONAL -
CD                            CASE.                                   -
CD     NCINTK             NUMBER OF THIRD DIMENSION COARSE MESH INTERVALS-
CD                            NCINTK.EQ.1 FOR ONE AND TWO DIMENSIONAL -
CD                            CASES.                                  -
CD     NINTI              NUMBER OF FIRST DIMENSION FINE MESH INTERVALS -
CD     NINTJ              NUMBER OF SECOND DIMENSION FINE MESH INTERVALS -
CD                            NINTJ.EQ.1 FOR ONE DIMENSIONAL CASE.    -
CD     NINTK              NUMBER OF THIRD DIMENSION FINE MESH INTERVALS -
CD                            NINTK.EQ.1 FOR ONE AND TWO DIMENSION CASES.-
CD     IMB1               FIRST BOUNDARY ON FIRST DIMENSION           -
CD                            0 - ZERO FLUX (DIFFUSION)               -
CD                            1 - REFLECTED                           -
CD                            2 - EXTRAPOLATED (DIFFUSION - DEL PHI/PHI -
CD                                = -C/D WHERE C IS GIVEN AS BNDC BELOW -
CD                                AND D IS THE GROUP DIFFUSION CONSTANT, -
CD                                TRANSPORT - NO RETURN).           -
CD                            3 - REPEATING (PERIODIC) WITH OPPOSITE FACE-
CD                            4 - REPEATING (PERIODIC) WITH NEXT ADJACENT-
CD                                FACE.                             -
CD                            5 - INVERTED REPEATING ALONG THIS FACE.   -
CD                                (180 DEGREE ROTATION)             -
CD                            6 - ISOTROPIC RETURN (TRANSPORT)        -
C                                                                     -
CC          NOTE FOR REPEATING CONDITIONS (3,4,5) - LET I1 DENOTE FIRST-
CC          BOUNDARY ON FIRST DIMENSION, I2 THE SECOND BOUNDARY ON THE -
CC          FIRST DIMENSION, J1 THE FIRST BOUNDARY ON THE SECOND      -
CC          DIMENSION, ETC. THEN THESE REPEATING BOUNDARY CONDITIONS   -
CC          ONLY APPLY TO BOUNDARIES I1,I2,J1, AND J2. GOING IN ORDER -
CC          OF I1,J1,I2,J2, THE FIRST BOUNDARY WHICH IS INVOLVED      -
CC          CARRIES THE DESIGNATOR DEFINING THE REPEATING CONDITION.  -
C                                                                     -
CD     IMB2                    LAST BOUNDARY ON FIRST DIMENSION       -
CD     JMB1                    FIRST BOUNDARY ON SECOND DIMENSION     -
CD     JMB2                    LAST BOUNDARY ON SECOND DIMENSION      -
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C     KMB1            FIRST BOUNDARY ON THIRD DIMENSION                -
C     KMB2            LAST BOUNDARY ON THIRD DIMENSION                 -
C     NBS             NUMBER OF BUCKLING SPECIFICATIONS                -
C                         0 - NONE                                     -
C                         1 - SINGLE VALUE APPLIES EVERYWHERE          -
C                         .EQ.NZONE-  ZONE DEPENDENT                   -
C                         M*NZONE - DATA IS GIVEN OVER ALL ZONES FOR   -
C                             THE FIRST ENERGY GROUP, THEN FOR THE     -
C                             NEXT GROUP, TO END OF LIST.  IF          -
C                             M.LT.NGROUP THEN THE M-TH GROUP DATA     -
C                             APPLIES TO ALL ADDITIONAL GROUPS.        -
C                             (2.LE.M.LE.NGROUP)                       -
C     NBCS            NUMBER OF CONSTANTS FOR EXTERNAL BOUNDARIES      -
C                         0 - NONE                                     -
C                         1 - SINGLE VALUE USED EVERYWHERE             -
C                         6 - INDIVIDUAL VALUE GIVEN FOR EACH          -
C                             EXTERNAL BOUNDARY. THE ORDERING OF THE   -
C                             VALUES IS THE SAME AS THE ORDERING OF    -
C                             THE BOUNDARY CONDITIONS.                 -
C                         6*M - SIX VALUES GIVEN FOR FIRST ENERGY      -
C                             GROUP (ORDERED AS DESCRIBED ABOVE),      -
C                             THEN 6 FOR THE NEXT GROUP, TO END OF     -
C                             LIST.  (2.LE.M.LE.NGROUP).               -
C                             IF M.LT.NGROUP THEN THE M-TH GROUP DATA- -
C                             APPLIES TO ALL REMAINING GROUPS.         -
C     NIBCS           NUMBER OF CONSTANTS FOR INTERNAL BOUNDARIES      -
C                         0 - NONE                                     -
C                         1 - SINGLE VALUE USED EVERYWHERE             -
C                         .GT.1 - VALUES ARE GIVEN BY ENERGY GROUP     -
C                           WITH NON-BLACK CONDITION INDICATED BY      -
C                           ZERO ENTRY - LAST VALUE APPLIES TO         -
C                           ADDITIONAL GROUPS                          -
C     NZWBB           NUMBER OF ZONES WHICH ARE BLACK ABSORBERS        -
C     NTRIAG          TRIANGULAR/HEXAGONAL GEOMETRY OPTION             -
C                         0 - REGION OF SOLUTION IS A RHOMBUS IN       -
C                             WHICH THE 1ST AND 2ND DIMENSION AXES     -
C                             INTERSECT AT AN ANGLE OF 120 DEGREES.    -
C                         1 - REGION OF SOLUTION IS A RHOMBUS IN       -
C                             WHICH THE 1ST AND 2ND DIMENSION AXES     -
C                             INTERSECT AT AN ANGLE OF 60 DEGREES.     -
C                         2 - REGION OF SOLUTION IS A RECTANGLE.  THE- -
C                             BOUNDARIES I1 AND I2 BISECT MESH         -
C                             TRIANGLES.  SEE NTHPT BELOW.             -
C                             (IGOM=9,17 ONLY)                         -
C                         3 - REGION OF SOLUTION IS AN EQUILATERAL,    -
C                             60 DEGREE TRIANGLE.  (IGOM=9,17 ONLY)    -
C                         4 - REGION OF SOLUTION IS A 30-60 DEGREE     -
C                             RIGHT TRIANGLE IN WHICH THE 1ST AND 2ND- -
C                             DIMENSION AXES INTERSECT AT THE 30       -
C                             DEGREE ANGLE.  (IGOM=9,17 ONLY)          -
C                         5 - REGION OF SOLUTION IS A RHOMBUS IN       -
C                             WHICH THE 1ST AND 2ND DIMENSION AXES     -
C                             INTERSECT AT AN ANGLE OF 30 DEGREES.     -
C                             (IGOM=9,17 ONLY)                         -
CD    NRASS           REGION ASSIGNMENTS                               -
CD                        0- TO COARSE MESH                            -
CD                        1- TO FINE MESH                              -
CD    NTHPT           ORIGIN OF FIRST FINE MESH INTERVAL IN            -
CD                        TRIANGULAR GEOMETRIES.  NTRIAG=2 ONLY.       -
CD                        ANGLE(1,1) POINTS AWAY FROM FIRST            -
CD                        DIMENSION AXIS, I.E., NO INTERNAL MESH       -
CD                        LINE INTERSECTS THE ORIGIN.                  -
CD                        ANGLE(1,1) POINTS TOWARD THE FIRST           -
CD                        DIMENSION AXIS, I.E., AN INTERNAL MESH       -
CD                        LINE INTERSECTS THE ORIGIN.                  -
CD    NGOP            RESERVED                                         -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          ONE DIMENSIONAL COARSE MESH INTERVAL BOUNDARIES AND FINE    -
CR          MESH INTERVALS (2D RECORD)                                  -
C                                                                       -
CC          PRESENT IF IGOM.GT.0 AND IGOM.LE.3                          -
C                                                                       -
CL    (XMESH(I),I=1,NCBNDI),(IFINTS(I),I=1,NCINTI)                      -
C                                                                       -
CW    NCBNDI*MULT+NCINTI                                                -
C                                                                       -
CD    XMESH           COARSE MESH BOUNDARIES, FIRST DIMENSION           -
CD    IFINTS          NUMBER OF EQUALLY SPACED FINE MESH INTERVALS      -
CD                        PER COARSE MESH INTERVAL, FIRST DIMENSION.    -
CD    NCBNDI          NCINTI+1, NUMBER OF FIRST DIMENSION COARSE MESH-  -
CD                        BOUNDARIES                                    -
C                                                                       -
CC        UNITS ARE CM FOR LINEAR DIMENSIONS AND RADIANS FOR ANGULAR    -
CC        DIMENSIONS                                                    -
C                                                                       -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          TWO DIMENSIONAL COARSE MESH INTERVAL BOUNDARIES AND FINE    -
CR          MESH INTERVALS (3D RECORD)                                  -
C                                                                       -
CC          PRESENT IF IGOM.GE.6 AND IGOM.LE.11                         -
C                                                                       -
CL    (XMESH(I),I=1,NCBNDI),(YMESH(J),J=1,NCBNDJ),                      -
CL   1(IFINTS(I),I=1,NCINTI),(JFINTS(J),J=1,NCINTJ)                     -
C                                                                       -
CW    (NCBNDI+NCBNDJ)*MULT+NCINTI+NCINTJ                                -
C                                                                       -
CD    YMESH           COARSE MESH BOUNDARIES, SECOND DIMENSION          -
CD    JFINTS          NUMBER OF EQUALLY SPACED FINE MESH INTERVALS      -
CD                        PER COARSE MESH INTERVAL, SECOND DIMENSION.-  -
CD    NCBNDJ          NCINTJ+1, NUMBER OF SECOND DIMENSION COARSE       -
CD                        MESH BOUNDARIES                               -
C                                                                       -
CC          FOR UNIFORM-TRIANGULAR-MESH GEOMETRY (IGOM = 9) THE         -
CC          LENGTH (L) OF THE SIDE OF A MESH TRIANGLE MUST BE GIVEN     -
CC          BY THE EXPRESSION                                           -
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CC                    L = 2.*(XMESH(2)-XMESH(1))/IFINTS(1) .
CC          FOR UNIFORM-HEXAGONAL-MESH GEOMETRY (IGOM = 10) THE
CC          FLAT-TO-FLAT DISTANCE (FTF) ACROSS A MESH HEXAGON MUST
CC          BE GIVEN BY THE EXPRESSION
CC                    FTF = (XMESH(2)-XMESH(1))/IFINTS(1)
C
C-----------------------------------------------------------------
C-----------------------------------------------------------------
CR          THREE DIMENSIONAL COARSE MESH INTERVAL BOUNDARIES AND FINE
CR          MESH INTERVALS (4D RECORD)
C
CC          PRESENT IF IGOM.GE.12
C
CL     (XMESH(I),I=1,NCBNDI),(YMESH(J),J=1,NCBNDJ),
CL    1(ZMESH(K),K=1,NCBNDK),(IFINTS(I),I=1,NCINTI),
CL    2(JFINTS(J),J=1,NCINTJ),(KFINTS(K),K=1,NCINTK)
C
CW     (NCBNDI+NCBNDJ+NCBNDK)*MULT+NCINTI+NCINTJ+NCINTK
C
CD     ZMESH               COARSE MESH BOUNDARIES, THIRD DIMENSION
CD     KFINTS              NUMBER OF EQUALLY SPACED FINE MESH INTERVALS
CD                             PER COARSE MESH INTERVAL, THIRD DIMENSION.
CD     NCBNDK              NCINTK+1, NUMBER OF THIRD DIMENSION COARSE MESH
CD                             BOUNDARIES
C
CC          FOR UNIFORM-TRIANGULAR-MESH GEOMETRY (IGOM = 17) THE
CC          LENGTH (L) OF THE SIDE OF A MESH TRIANGLE MUST BE GIVEN
CC          BY THE EXPRESSION
CC                    L = 2.*(XMESH(2)-XMESH(1))/IFINTS(1) .
CC          FOR UNIFORM-HEXAGONAL-MESH GEOMETRY (IGOM = 18) THE
CC          FLAT-TO-FLAT DISTANCE (FTF) ACROSS A MESH HEXAGON MUST
CC          BE GIVEN BY THE EXPRESSION
CC                    FTF = (XMESH(2)-XMESH(1))/IFINTS(1)
C
C-----------------------------------------------------------------
C-----------------------------------------------------------------
CR          GEOMETRY DATA (5D RECORD)
C
CC          PRESENT IF IGOM.GT.0 OR NBS.GT.0
C
CL     (VOLR(N),N=1,NREG),(BSQ(N),N=1,NBS),(BNDC(N),N=1,NBCS),
CL     (BNCI(N),N=1,NIBCS),((NZHBB(N),N=1,NZWBB),(NZC(N),N=1,NZONE),
CL     (NZNR(N),N=1,NREG)
C
CW     2*NREG+NBS+NBCS+NIBCS+NZWBB+NZONE
C
CD     VOLR                REGION VOLUMES (CC)
CD     BSQ                 BUCKLING (B**2) VALUES (CM**-2)
CD     BNDC                BOUNDARY CONSTANTS (DEL PHI/PHI =-C/D)
CD     BNCI                INTERNAL BLACK BOUNDARY CONSTANTS
CD     NZHBB               ZONE NUMBERS WITH BLACK ABSORBER CONDITIONS
CD     NZC                 ZONE CLASSIFICATIONS
CD     NZNR                ZONE NUMBER ASSIGNED TO EACH REGION
C
C-----------------------------------------------------------------
C-----------------------------------------------------------------
CR          REGION ASSIGNMENTS TO COARSE MESH INTERVALS (6D RECORD)
C
CC          PRESENT IF IGOM.GT.0 AND NRASS.EQ.0
C
CL     ((MR(I,J),I=1,NCINTI),J=1,NCINTJ)----NOTE STRUCTURE BELOW----
C
CW     NCINTI*NCINTJ
C
CS     DO 1 K=1,NCINTK
CS    1 READ(N) *LIST AS ABOVE*
C
CD     MR                  REGION NUMBERS ASSIGNED TO COARSE MESH
CD                             INTERVALS
C
C-----------------------------------------------------------------
C-----------------------------------------------------------------
CR          REGION ASSIGNMENTS TO FINE MESH INTERVALS (7D RECORD)
C
CC          PRESENT IF IGOM.GT.0 AND NRASS.EQ.1
C
CL     ((MR(I,J),I=1,NINTI),J=1,NINTJ)----NOTE STRUCTURE BELOW----
C
CW     NINTI*NINTJ
C
CS     DO 1 K=1,NINTK
CS    1 READ(N) *LIST AS ABOVE*
C
CD     MR                  REGION NUMBERS ASSIGNED TO FINE MESH INTERVALS
C
C-----------------------------------------------------------------
CEOF
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C.3 NDXSRF

```
C*****************************************************************************
C                         REVISED 11/30/76
C
CF          NDXSRF-IV
C
CE          NUCLIDE DENSITY, DATA, CROSS SECTION REFERENCING
C
C*****************************************************************************
C-----------------------------------------------------------------
CR          FILE IDENTIFICATION
C
CL     HNAME,(HUSE(I),I=1,2),IVERS
C
CW     1+3*MULT=NUMBER OF WORDS
C
CD     HNAME          HOLLERITH FILE NAME - NDXSRF - (A6)
```

```
CD    HUSE(I)        HOLLERITH USER IDENTIFICATION (A6)                -
CD    IVERS          FILE VERSION NUMBER                               -
CD    MULT           DOUBLE PRECISION PARAMETER                        -
CD                       1- A6 WORD IS SINGLE WORD                     -
CD                       2-A6 WORD IS DOUBLE PRECISION WORD            -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          SPECIFICATIONS          (1D RECORD)                        -
C                                                                      -
CL    NON,NSN,NNS,NAN,NZONE,NSZ                                        -
C                                                                      -
CW    6   =NUMBER OF WORDS                                             -
C                                                                      -
CD    NON              NUMBER OF NUCLIDES IN CROSS SECTION DATA        -
CD    NSN              NUMBER OF NUCLIDE SETS IDENTIFIED               -
CD    NNS              MAXIMUM NUMBER OF NUCLIDES IN ANY SET           -
CD    NAN              NUMBER OF DIFFERENT NUCLIDES IN DATA            -
CD    NZONE            NUMBER OF ZONES                                 -
CD    NSZ              NUMBER OF SUBZONES (SUBASSEMBLIES)              -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
C          NUCLIDE REFERENCING DATA       (2D RECORD)                 -
C                                                                      -
CL      (HNNAME(N),N=1,NON),(HANAME(N),N=1,NON),(WPF(N),N=1,NON),      -
CL    (ATWT(J),J=1,NAN),(NCLN(N),N=1,NON),((NDXS(K,L),K=1,4),L=1,NSN), -
CL    ((NOS(I,L),I=1,NNS),L=1,NSN),((NOR(N,L),N=1,NON),L=1,NSN)        -
C                                                                      -
CW  NAN+2*NON*(1+MULT)+NSN*(4+NNS+NON)=NUMBER OF WORDS                 -
C                                                                      -
CD    HNNAME(N)        UNIQUE REFERENCE NUCLIDE NAME, IN LIBRARY ORDER-
CD                        (A6) ALPHANUMERIC                           -
CD    HANAME(N)        ABSOLUTE NUCLIDE REFERENCE, IN LIBRARY ORDER    -
CD                        (A6) ALPHANUMERIC                           -
CD    WPF(N)           RESERVED                                        -
CD    ATWT(J)          ATOMIC WEIGHT                                   -
CD    NCLN(N)          NUCLIDE CLASSIFICATION                          -
CD                        1- FISSILE                                  -
CD                        2- FERTILE                                  -
CD                        3- OTHER ACTINIDE                           -
CD                        4- FISSION PRODUCT                          -
CD                        5- STRUCTURAL                               -
CD                        6- COOLANT                                  -
CD                        7- CONTROL ROD                              -
CD                        GREATER THAN 7, UNDEFINED                   -
CD    NDXS(K,L)        REFERENCE DATA FOR SET L                        -
CD                        K = 1, NUMBER OF NUCLIDES IN SET            -
CD                        K = 2, RESERVED                             -
CD                        K = 3, RESERVED                             -
CD                        K = 4, RESERVED                             -
CD    NOS(I,L)         ORDER NUMBER OF NUCLIDE IN CROSS SECTION DATA   -
CD                        (IN HNNAME LIST) OF NUCLIDE ORDERED I IN    -
CD                        SET L                                       -
CD    NOR(N,L)         ORDER NUMBER OF NUCLIDE IN SET L GIVEN ORDER    -
CD                        NUMBER N IN CROSS SECTION DATA               -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
C          NUCLIDE CONCENTRATION ASSIGNMENT DATA     (3D RECORD)       -
C                                                                      -
CL    (VOLZ(N),N=1,NZONE),(VFPA(N),N=1,NZONE),(VLSA(M),M=1,NSZ),       -
CL    (NSPA(N),N=1,NZONE),(NSSA(M),M=1,NSZ),(NZSZ(M),M=1,NSZ)          -
C                                                                      -
CW    3*(NZONE+NSZ)=NUMBER OF WORDS                                    -
C                                                                      -
CD    VOLZ(N)          VOLUMES OF ZONES, CC                            -
CD    VFPA(N)          VOLUME FRACTIONS FOR PRIMARY ZONE ASSIGNMENTS   -
CD    VLSA(M)          VOLUMES OF SUBZONES                             -
CD    NSPA(N)          NUCLIDE SET REFERENCE, PRIMARY ZONE ASSIGNMENT  -
CD                        (MAY BE ZERO ONLY IF THERE ARE SUBZONES)     -
CD    NSSA(M)          NUCLIDE SET REFERENCE ASSIGNMENT TO SUBZONES    -
CD    NZSZ(M)          ZONE CONTAINING SUBZONE                         -
C                                                                      -
C     NOTE THAT TO CALCULATE MACROSCOPIC CROSS SECTIONS FOR A ZONE,    -
C     IT IS NECESSARY TO CONSIDER THE CONCENTRATION OF EACH NUCLIDE    -
C     IN THE PRIMARY SET ASSIGNMENT (UNLESS A ZERO IN NSPA INDICATES   -
C     THERE ARE NONE) TIMES THE VOLUME FRACTION, AND THE CONCENTRATION -
C     OF EACH NUCLIDE IN EACH SUBZONE ASSIGNED TO THE ZONE TIMES THE   -
C     RATIO OF THE SUBZONE VOLUME TO THE ZONE VOLUME.                  -
C                                                                      -
C----------------------------------------------------------------------
CEOF
```

C.4 ZNATDN

```
C**********************************************************************
C                         REVISED 11/30/76                             -
C                                                                      -
CF          ZNATDN-IV                                                  -
C                                                                      -
CE          ZONE ATOMIC DENSITIES (OF NUCLIDES)                        -
C                                                                      -
C**********************************************************************
C----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
CD    HNAME            HOLLERITH FILE NAME - ZNATDN -(A6)              -
CD    HUSE(I)          HOLLERITH USER IDENTIFICATION (A6)              -
CD    IVERS            FILE VERSION NUMBER                             -
CD    MULT             DOUBLE PRECISION PARAMETER                      -
CD                        1- A6 WORD IS SINGLE WORD                    -
```

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CD                        2- A6 WORD IS DOUBLE PRECISION WORD
C
C-------------------------------------------------------------------
C-------------------------------------------------------------------
CR          SPECIFICATIONS          (1D RECORD)
C
CL    TIME,NCY,NTZSZ,NNS,NBLKAD
C
CW    5=NUMBER OF WORDS
C
CD    TIME              REFERENCE REAL TIME, DAYS
CD    NCY               REFERENCE CYCLE NUMBER
CD    NTZSZ             NUMBER OF ZONES PLUS NUMBER OF SUBZONES
CD    NNS               MAXIMUM NUMBER OF NUCLIDES IN ANY SET
CD    NBLKAD            NUMBER OF BLOCKS OF ATOM DENSITY DATA
C
C-------------------------------------------------------------------
C-------------------------------------------------------------------
CR          ZONE ATOMIC DENSITIES (OF NUCLIDES)      (2D RECORD)
C
CL    ((ADEN(N,J),N=1,NNS),J=JL,JU)----SEE STRUCTURE BELOW----
C
CW    NNS*(JL - JU + 1) = NUMBER OF WORDS
C
CC    DO 1 M=1,NBLKAD
CC  1 READ(N) *LIST AS ABOVE*
C
CC        WITH M AS THE BLOCK INDEX, JL=(M-1)*((NTZSZ-1)/NBLKAD+1)+1
CC        AND JU=MINO(NTZSZ,JUP) WITH JUP=M*((NTZSZ-1)/NBLKAD + 1)
C
CD    ADEN(N,J)         ATOMIC DENSITY OF NUCLIDE ORDERED N IN THE
CD                      ASSOCIATED SET GIVEN IN ORDER FOR EACH ZONE
CD                      FOLLOWED IN ORDER FOR EACH SUBZONE
C
C-------------------------------------------------------------------
CEOF
```

C.5 FIXSRC

```
C*******************************************************************
C                       REVISED 11/30/76
C
CF          FIXSRC-IV
CE          DISTRIBUTED AND SURFACE FIXED SOURCES
C
C*******************************************************************
C-------------------------------------------------------------------
CR          FILE IDENTIFICATION
C
CL    HNAME,(HUSE(I),I=1,2),IVERS
C
CW    1+3*MULT=NUMBER OF WORDS
C
CD    HNAME             HOLLERITH FILE NAME - FIXSRC - (A6)
CD    HUSE(I)           HOLLERITH USER IDENTIFICATION (A6)
CD    IVERS             FILE VERSION NUMBER
CD    MULT              DOUBLE PRECISION PARAMETER
CD                          1- A6 WORD IS SINGLE WORD
CD                          2- A6 WORD IS DOUBLE PRECISION WORD
C
C-------------------------------------------------------------------
C-------------------------------------------------------------------
CR          SPECIFICATIONS   (1D RECORD)
C
CL    ITYPE,NDIM,NGROUP,NINTI,NINTJ,NINTK,IDISTS,NDCOMP,NSCOMP,NEDGI,
CL    NEDGJ,NEDGK,NBLOK
C
CW    13=NUMBER OF WORDS
C
CD    ITYPE             TYPE SOURCE. 0=DIFFUSION
CD                                   1=SN
CD    NDIM              NUMBER OF  DIMENSIONS
CD    NGROUP            NUMBER OF GROUPS
CD    NINTI             NUMBER OF FIRST DIMENSION FINE MESH INTERVALS
CD    NINTJ             NUMBER OF SECOND DIMENSION FINE MESH INTERVALS
CD    NINTK             NUMBER OF THIRD DIMENSION FINE MESH INTERVALS
CD    IDISTS            DISTRIBUTED SOURCE FLAG.
CD                          0= NO DISTRIBUTED SOURCE GIVEN.
CD                          1= DISTRIBUTED SOURCE IS GIVEN.
CD    NDCOMP            NUMBER OF DISTRIBUTED SOURCE COMPONENTS
CD    NSCOMP            NUMBER OF SURFACE SOURCE COMPONENTS
CD    NEDGI             NUMBER OF FIRST DIMENSION BOUNDARY  SOURCES
CD    NEDGJ             NUMBER OF SECOND DIMENSION  BOUNDARY SOURCES
CD    NEDGK             NUMBER OF THIRD DIMENSION BOUNDARY SOURCES
CD    NBLOK             DATA BLOCKING FACTOR FOR DISTRIBUTED FIXED
CD                       SOURCES IN MULTI-DIMENSIONS. (2ND DIMENSION
CD                       VARIABLE IS BLOCKED INTO NBLOK BLOCKS,
CD                       SEE 3D RECORD BELOW)
C
C-------------------------------------------------------------------
C-------------------------------------------------------------------
CR          ONE-DIMENSIONAL DISTRIBUTED FIXED SOURCE  (2D RECORD)
C
CC          PRESENT IF NDIM.EQ.1 AND IDISTS.NE.0
C
CL    ((QDIST(L,I),L=1,NDCOMP),I=1,NINTI)---NOTE STRUCTURE BELOW---
C
CW    NDCOMP*NINTI=NUMBER OF WORDS
C
C     DO 1 J=1,NGROUP
C   1 READ (N) *LIST AS ABOVE*
C
CD    QDIST(L,I)        DISTRIBUTED SOURCE BY COMPONENT, INTERVAL,
CD                      AND GROUP
C
C-------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR          MULTI-DIMENSIONAL DISTRIBUTED FIXED SOURCE  (3D RECORD)     -
C                                                                        -
CC          PRESENT IF NDIM.GE.2 AND IDISTS.NE.0                         -
C                                                                        -
CL    ((QDIST(I,J),I=1,NINTI),J=JL,JU) ------SEE STRUCTURE BELOW------   -
C                                                                        -
CW    NINTI*(JU - JL + 1) = NUMBER OF WORDS                              -
C                                                                        -
C     DO 1 N=1,NGROUP                                                    -
C     DO 1 L=1,NDCOMP                                                    -
C     DO 1 K=1,NINTK                                                     -
C     DO 1 M=1,NBLOK                                                     -
C   1 READ (N) *LIST AS ABOVE*                                           -
C                                                                        -
CC          WITH M AS THE BLOCK INDEX, JL=1+(M-1)*((NINTJ-1)/NBLOK +1)  -
CC          AND JU=MIN0(NINTJ,JUP) WHERE JUP=M*((NINTJ-1)/NBLOK +1)     -
C                                                                        -
CD    QDIST(I,J)          DISTRIBUTED SOURCE AS DEFINED ABOVE            -
C                                                                        -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          FIRST DIMENSION SURFACE SOURCE POINTERS   (4D RECORD)        -
C                                                                        -
CC          PRESENT IF NEDGI.NE.0                                        -
C                                                                        -
CL    ((ISPTRI(I,J),I=1,NBDRYI),J=1,NINTJ)---NOTE STRUCTURE BELOW---     -
C                                                                        -
CW    NBDRYI*NINTJ=NUMBER OF WORDS                                       -
C                                                                        -
C     DO 1 K=1,NINTK                                                     -
C   1 READ (N) *LIST AS ABOVE*                                           -
C                                                                        -
CD    ISPTRI(I,J)         ISPTRI(I,J) DENOTES THE INTERCEPT OF CHANNEL   -
CD                        J,K WITH MESH BOUNDARY PLANE I.  IF ISPTRI(I,J)-
CD                        =0, NO SURFACE SOURCE IS PRESENT AT THE        -
CD                        INTERCEPT.  IF ISPTRI(I,J)=M, THE MTH SURFACE  -
CD                        SOURCE SPECIFIED IN THE NEXT RECORD BELOW IS   -
CD                        PRESENT AT THE INTERCEPT.                      -
CD    NBDRYI              =NINTI+1, NUMBER OF FIRST DIMENSION FINE MESH  -
CD                         BOUNDARIES                                    -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          FIRST DIMENSION SURFACE SOURCES    (5D RECORD)               -
C                                                                        -
CC          PRESENT IF NEDGI.NE.0                                        -
C                                                                        -
CL    (((QSURFI(M,L,N),M=1,NEDGI),L=1,NSCOMP),N=1,NGROUP)                -
C                                                                        -
CW    NEDGI*NGROUP*NSCOMP=NUMBER OF WORDS                                -
C                                                                        -
CD    QSURFI(M,L,N)       FIRST DIMENSION BOUNDARY SOURCES BY BOUNDARY,  -
CD                        COMPONENT, AND GROUP.                          -
C                                                                        -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          SECOND DIMENSION SURFACE SOURCE POINTERS   (6D RECORD)       -
C                                                                        -
C           PRESENT IF NDIM.GE.2 AND NEDGJ.NE.0                          -
C                                                                        -
CL    ((ISPTRJ(I,J),I=1,NINTI),J=1,NBDRYJ)---NOTE STRUCTURE BELOW---     -
C                                                                        -
CW    NINTI*NBDRYJ=NUMBER OF WORDS                                       -
C                                                                        -
C     DO 1 K=1,NINTK                                                     -
C   1 READ (N) *LIST AS ABOVE*                                           -
C                                                                        -
CD    ISPTRJ(I,J)         ISPTRJ(I=J) DENOTES THE INTERCEPT OF CHANNEL   -
CD                        I,K WITH MESH BOUNDARY PLANE J.  IF ISPTRJ(I,J)-
CD                        =0, NO SURFACE SOURCE IS PRESENT AT THE        -
CD                        INTERCEPT.  IF ISPTRJ(I,J)=M, THE MTH SURFACE  -
CD                        SOURCE SPECIFIED IN THE NEXT RECORD BELOW IS   -
CD                        PRESENT AT THE INTERCEPT.                      -
CD    NBDRYJ              =NINTJ+1, NUMBER OF SECOND DIMENSION FINE MESH -
CD                        BOUNDARIES                                     -
C                                                                        -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          SECOND DIMENSION SURFACE SOURCES   (7D RECORD)               -
C                                                                        -
CC          PRESENT IF NDIM.GE.2 AND NEDGJ.NE.0                          -
C                                                                        -
CL    (((QSURFJ(M,L,N),M=1,NEDGJ),L=1,NSCOMP),N=1,NGROUP)                -
C                                                                        -
CW    NEDGJ*NGROUP*NSCOMP=NUMBER OF WORDS                                -
C                                                                        -
CD    QSURFJ(M,L,N)       SECOND DIMENSION BOUNDARY SOURCES BY BOUNDARY  -
CD                        COMPONENT, AND GROUP                           -
C                                                                        -
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          THIRD DIMENSION SURFACE SOURCE POINTERS   (8D RECORD)        -
C                                                                        -
CC          PRESENT IF NDIM.EQ.3 AND NEDGK.NE.0                          -
C                                                                        -
CL    ((ISPTRK(I,J),I=1,NINTI),J=1,NINTJ)---NOTE STRUCTURE BELOW---      -
C                                                                        -
CW    NINTI*NINTJ=NUMBER OF WORDS                                        -
C                                                                        -
C     DO 1 K=1,NBDRYK                                                    -
C   1 READ (N) *LIST AS ABOVE*                                           -
C                                                                        -
CD    ISPTRK(I,J)         ISPTRK(I,J) DENOTES THE INTERCEPT OF CHANNEL   -
CD                        I,J WITH MESH BOUNDARY PLANE K.  IF ISPTRK(I,J)-
CD                        =0, NO SURFACE SOURCE IS PRESENT AT THE        -
CD                        INTERCEPT.  IF ISPTRK(I,J)=M, THE MTH SURFACE  -
CD                        SOURCE SPECIFIED IN THE NEXT RECORD BELOW IS   -
CD                        PRESENT AT THE INTERCEPT.                      -
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CD    NBDRYK              =NINTK+1, NUMBER OF THIRD DIMENSION FINE MESH -
CD                         BOUNDARIES                                  -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          THIRD DIMENSION SURFACE SOURCES     (9D RECORD)            -
C                                                                      -
CC          PRESENT IF NDIM.EQ.3 AND NEDGK.NE.0                        -
C                                                                      -
CL    (((QSURFK(M,L,N),M=1,NEDGK),L=1,NSCOMP),N=1,NGROUP)              -
C                                                                      -
CW    NEDGK*NGROUP*NSCOMP=NUMBER OF WORDS                              -
C                                                                      -
CD    QSURFK(M,L,N)       THIRD DIMENSION BOUNDARY SOURCES BY BOUNDARY, -
CD                        COMPONENT, AND GROUP                         -
C                                                                      -
C----------------------------------------------------------------------
CEOF
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C.6 RTFLUX

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C**********************************************************************
C                         REVISED 11/30/76                             -
C                                                                      -
CF          RTFLUX-IV                                                  -
CE          REGULAR TOTAL FLUXES                                       -
C                                                                      -
C**********************************************************************
CD                        ORDER OF GROUPS IS ACCORDING TO DECREASING
CD                        ENERGY. NOTE THAT DOUBLE PRECISION FLUXES ARE
CD                        GIVEN WHEN MULT=2
C----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
CD    HNAME               HOLLERITH FILE NAME - RTFLUX - (A6)          -
CD    HUSE(I)             HOLLERITH USER IDENTIFICATION (A6)           -
CD    IVERS               FILE VERSION NUMBER                          -
CD    MULT                DOUBLE PRECISION PARAMETER                   -
CD                            1- A6 WORD IS SINGLE WORD                -
CD                            2- A6 WORD IS DOUBLE PRECISION WORD      -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          SPECIFICATIONS      (1D RECORD)                            -
C                                                                      -
CL    NDIM,NGROUP,NINTI,NINTJ,NINTK,ITER,EFFK,POWER,NBLOK              -
C                                                                      -
CW    9 =NUMBER OF WORDS                                               -
C                                                                      -
CD    NDIM                NUMBER OF DIMENSIONS                         -
CD    NGROUP              NUMBER OF ENERGY GROUPS                      -
CD    NINTI               NUMBER OF FIRST DIMENSION FINE MESH INTERVALS -
CD    NINTJ               NUMBER OF SECOND DIMENSION FINE MESH INTERVALS -
CD    NINTK               NUMBER OF THIRD DIMENSION FINE MESH INTERVALS. -
CD                        NINTK.EQ.1 IF NDIM.LE.2                      -
CD    ITER                OUTER ITERATION NUMBER AT WHICH FLUX WAS     -
CD                        WRITTEN                                      -
CD    EFFK                EFFECTIVE MULTIPLICATION FACTOR              -
CD    POWER               POWER IN WATTS TO WHICH FLUX IS NORMALIZED    -
CD    NBLOK               DATA BLOCKING FACTOR                         -
CD                           IF NDIM.EQ.1 THE GROUP VARIABLE IS BLOCKED -
CD                              INTO NBLOK BLOCKS (SEE 2D RECORD BELOW) -
CD                           IF NDIM.GE.2 THE 2ND DIMENSION VARIABLE IS -
CD                              BLOCKED INTO NBLOK BLOCKS (SEE 3D RECORD)-
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          ONE DIMENSIONAL REGULAR TOTAL FLUX   (2D RECORD)           -
C                                                                      -
CC          PRESENT IF NDIM.EQ.1                                       -
C                                                                      -
CL    ((FREG(I,J),I=1,NINTI),J=JL,JU)-----SEE STRUCTURE BELOW-----     -
C                                                                      -
CW    NINTI*(JU - JL + 1)*MULT = NUMBER OF WORDS                       -
C                                                                      -
C     DO 1 M=1,NBLOK                                                   -
C   1 READ(N)   *LIST AS ABOVE*                                        -
C                                                                      -
CC          WITH M AS THE BLOCK INDEX, JL=(M-1)*((NGROUP-1)/NBLOK+1)+1 -
CC          AND JU=MINO(NGROUP,JUP) WHERE JUP=M*((NGROUP-1)/NBLOK +1)  -
C                                                                      -
CD    FREG(I,J)           ONE DIMENSIONAL REGULAR TOTAL FLUX BY INTERVAL -
CD                        AND GROUP.                                   -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          MULTI-DIMENSIONAL REGULAR TOTAL FLUX   (3D RECORD)         -
C                                                                      -
CC          PRESENT IF NDIM.GE.2                                       -
C                                                                      -
CL    ((FREG(I,J),I=1,NINTI),J=JL,JU)-----SEE STRUCTURE BELOW-----     -
C                                                                      -
CW    NINTI*(JU - JL + 1)*MULT = NUMBER OF WORDS                       -
C                                                                      -
C     DO 1 L=1,NGROUP                                                  -
C     DO 1 K=1,NINTK                                                   -
C     DO 1 M=1,NBLOK                                                   -
C   1 READ(N)   *LIST AS ABOVE*                                        -
C                                                                      -
CC          WITH M AS THE BLOCK INDEX, JL=(M-1)*((NINTJ-1)/NBLOK +1)+1 -
CC          AND JU=MINO(NINTJ,JUP) WHERE JUP=M*((NINTJ-1)/NBLOK +1)    -
C                                                                      -
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CD    FREG(I,J)          MULTI-DIMENSIONAL REGULAR TOTAL FLUX          -
CD                       BY INTERVAL AND GROUP.                        -
C                                                                      -
C----------------------------------------------------------------------
CEOR
```

C.7 SEARCH

```
C**********************************************************************
C                        REVISED 03/09/81                              -
C                                                                      -
CF          SEARCH -IV (ANL)                                           -
C                                                                      -
CE          CRITICALITY SEARCH FILE                                    -
C                                                                      -
CC          THIS VERSION OF THE SEARCH FILE INDICATES THE SEARCH       -
CC          OPTIONS CURRENTLY IMPLEMENTED IN THE CRITICALITY SEARCH    -
CC          OPTION AT ARGONNE NATIONAL LABORATORY.  EXISTING OPTIONS   -
CC          WHICH DO NOT APPLY ARE INDICATED BY *N.A.*. NEW OPTIONS    -
CC          ARE INDICATED BY *NEW*.  MODIFICATIONS ARE INDICATED BY    -
CC          *MOD* OR BY A STRING OF CHARACTERS DELIMITED BY ASTERISKS.  -
CC          THIS RESTRICTED SUBSET OF THE SEARCH FILE OPTIONS IS       -
CC          COMPATIBLE WITH THE ORIGINAL SEARCH FILE (WITH THE         -
CC          EXCEPTION OF THE BUCKLING MODIFIERS RECORD WHICH DID NOT   -
CC          PREVIOUSLY EXIST).                                         -
C                                                                      -
C**********************************************************************
```

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C----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS             RECORD TYPE                          PRESENT IF         -
CS          ------------------------------------    ---------------    -
CS             FILE IDENTIFICATION                  ALWAYS             -
CS           *******(REPEAT UNTIL NSHID.LT.0)                         -
CS           *    INDIVIDUAL DATASET IDENTIFIER    ALWAYS             -
CS           *    FILE SPECIFICATIONS              NSHID.GT.0         -
CS           *    COARSE MESH MODIFIERS            NSHID.GT.0,ISRCH=5 -
CS           *    NUCLIDES FOR PROPORTIONAL SEARCH NSHID.GT.0,ISRCH=7 -
CS           *    NUCLIDES FOR SEARCH INVOLVING                      -
CS           *     WEIGHTED EIGENVALUE ADJUSTMENTS                   -
CS           *     TO INITIAL CONCENTRATIONS       NSHID.GT.0,ISRCH=9 -
CS *NEW*     *    COMPOSITION DEPENDENT BUCKLING                     -
CS           *     MODIFIERS                       NSHID.GT.0,ISRCH=1 -
CS           *******                                                  -
C                                                                      -
C----------------------------------------------------------------------
C----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
CD    HNAME              HOLLERITH FILE NAME - SEARCH - (A6)           -
CD    HUSE(I)            HOLLERITH USER IDENTIFICATION (A6)            -
CD    IVERS              FILE VERSION NUMBER                           -
CD    MULT               DOUBLE PRECISION PARAMETER                    -
CD                           1- A6 WORD IS SINGLE WORD                 -
CD                           2- A6 WORD IS DOUBLE PRECISION WORD       -
C                                                                      -
C----------------------------------------------------------------------
```

```
C----------------------------------------------------------------------
CR          INDIVIDUAL DATA SET IDENTIFIER       (1D RECORD)           -
C                                                                      -
CL    NSHID,NREC,(NSP(I),I=1,8),(SP(I),I=1,10)                         -
C                                                                      -
CW    20=NUMBER OF WORDS                                               -
C                                                                      -
CD    NSHID              POSITIVE INTEGER IDENTIFYING A SET OF SEARCH  -
CD                           DATA. THIS AND FOLLOWING RECORDS REPEATED -
CD                           UNTIL NEGATIVE NSHID TERMINATES FILE      -
CD    NREC               NUMBER OF RECORDS TO SKIP TO POSITION ON NEXT -
CD                           INDIVIDUAL DATA SET IDENTIFIER RECORD     -
CD    NSP(I)             RESERVED                                      -
CD    SP(1)      *MOD*   AVERAGE TIME IN SECONDS/SEARCH PASS
CD    SP(2)      *MOD*   TIME REMAINING AT THE START OF THE PREVIOUS
CD                       SEARCH PASS.
CD    SP(I)      *MOD*   RESERVED                                      -
C                                                                      .
C----------------------------------------------------------------------
```

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C----------------------------------------------------------------------
CR          FILE SPECIFICATIONS       (2D RECORD)                      -
C                                                                      -
CL    EFFK,DKEFF,EPSK,EPSEI,CMOD,(SRCH(I),I=1,5),ISRCH,ISZOP,NMAXNP,   -
CL    NCINTI,NCINTJ,NCINTK,NISOSR,NSETS,NEIRNG,ITEND,ICEND,            -
CL    (NRCH(I),I=1,10),(SRCH1(I),I=1,9)                                -
C                                                                      -
CW    40=NUMBER OF WORDS                                               -
C                                                                      -
CD    EFFK               DESIRED MULTIPLICATION FACTOR                 -
CD    DKEFF              USER SPECIFIED MULTIPLICATION FACTOR SLOPE     -
CD    EPSK               CONVERGENCE CRITERION TO BE MET BY EFFK        -
CD    EPSEI      *N.A.*  CONVERGENCE CRITERION TO BE MET BY PRIMARY     -
CD                           VARIABLE                                  -
CD    CMOD       *MOD*   MODIFIER APPLIED TO ALPHA (ISRCH=2) OR        -
CD                       MODIFIER APPLIED TO NUCLIDE CONCENTRATIONS     -
CD                           VARIED SPECIALLY (ISRCH=7 BELOW),MAY BE   -
CD                           .LT.0                                     -
CD    SRCH(1)  *EI(1)*   PREVIOUS PASS-1 SEARCH PARAMETER (EI)         -
CD    SRCH(2)  *EI(2)*   PREVIOUS PASS SEARCH PARAMETER (EI)           -
CD    SRCH(3)  *EI(3)*   MOST RECENT SEARCH PARAMETER (EI)             -
CD    SRCH(4)  *EIMIN*   USER SPECIFIED LOWER BOUND FOR SEARCH PARAMETER-
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CD                                (EI)                                          -
CD     SRCH(5)   *EIMAX*  USER SPECIFIED UPPER BOUND FOR SEARCH PARAMETER-
CD                                (EI)                                          -
CD     ISRCH              TYPE OF SEARCH                                        -
CD                            0- NOT DEFINED                                    -
CD                            1- BUCKLING SEARCH                                -
CD                            2- ALPHA SEARCH                                   -
CD                            5- DIMENSION SEARCH                               -
CD                            7- NUCLIDE CONCENTRATION SEARCH BY                -
CD                               PROPORTIONAL ADJUSTMENTS OF SELECTED           -
CD                               INITIAL CONCENTRATIONS                         -
CD                 *N.A.*     9- NUCLIDE CONCENTRATION SEARCH BY ADDING         -
CD                               WEIGHTED EIGENVALUE ADJUSTMENTS                -
CD                               TO SELECTED INITIAL CONCENTRATIONS             -
CD     ISZOP              SUBZONE OPTION FOR ISRCH = 7 OR 9                     -
CD                 *N.A.*     0- SEARCH DATA IS BY ZONE                         -
CD                            1- SEARCH DATA IS BY SUBZONE                      -
CD     NMAXNP     *GT 0*  MAXIMUM NUMBER OF NEUTRONICS PROBLEMS OR TRIAL -
CD                *ONLY*     EIGENVALUES ALLOWED IN A SEARCH. A ZERO           -
CD                            HERE SPECIFIES A DIRECT SEARCH.                   -
CD     NCINTI             NUMBER OF FIRST DIMENSION COARSE MESH INTERVALS-
CD     NCINTJ             NUMBER OF SECOND DIMENSION COARSE MESH                -
CD                            INTERVALS                                         -
CD     NCINTK             NUMBER OF THIRD DIMENSION COARSE MESH INTERVALS-
CD     NISOSR    *=NNS*   NUMBER OF ISOTOPES OR NUCLIDES INVOLVED IN            -
CD                *ONLY*     CONCENTRATION SEARCH (ISRCH = 7 OR 9)             -
CD     NSETS              NUMBER OF SPECIFICATION SETS IN CONCENTRATION         -
CD                            SEARCH (ISRCH = 7 OR 9)                           -
CD     NEIRNG             EIGENVALUE (EI) RANGE RESTRICTIONS. SEARCH            -
CD                            TERMINATED IF SPECIFIED RANGE IS VIOLATED.        -
CD                            -1  EI.LT.0                                       -
CD                             0- NO RESTRICTION ON EI                          -
CD                 *MOD*       1- EI.GT.EIMIN AND EI.LT.EIMAX                   -
CD                             2- EI.GT.1                                       -
CD     ITEND              TERMINATION OPTION ON ITERATIVE PROCESS. SEARCH-
CD                            IS LIMITED BY NMAXNP,NUMBER OF OUTER              -
CD                            ITERATIONS,OR OTHER PARAMETER,THEN                -
CD                            0- NO RESTRAINT                                   -
CD                 *N.A.*     1- TERMINATE IF CONVERGENCE CRITERIA ARE          -
CD                               NOT MET                                        -
CD                 *N.A.*     2- IF CONVERGENCE CRITERIA ARE NOT MET,           -
CD                               TERMINATE ONLY IF PROBLEM IS NOT               -
CD                               CONVERGING.                                    -
CD     ICEND              TERMINATION OPTIONS ON NUCLIDE CONCENTRATIONS         -
CD                 *N.A.*     0- TERMINATE IF ANY NUCLIDE CONCENTRATION         -
CD                               BECOMES NEGATIVE AT ANY STAGE OF THE           -
CD                               CALCULATION                                    -
CD                 *N.A.*     1- TERMINATE IF ANY NUCLIDE CONCENTRATION         -
CD                               IS NEGATIVE AT THE END OF THE SEARCH           -
CD                            2- ALLOW NEGATIVE NUCLIDE CONCENTRATIONS          -
CD     NRCH(1)   *NPASS*  SEARCH PASS NUMBER, INITIALLY 0                       -
CD     NRCH(2)   *NZONE*  NUMBER OF ZONES (ISRCH = 1)                           -
CD     NRCH(3)   *IEDTP*  SEARCH PARAMETER EDIT OPTION                          -
CD                        TWO DIGIT NUMBER (IF) WHERE                           -
CD                                                                              -
CD                        I CONTROLS INTERMEDIATE PASS PARAMETER EDITS          -
CD                        F CONTROLS FINAL PASS PARAMETER EDITS                 -
CD                                                                              -
CD                        THE INTEGERS I AND F ARE ASSIGNED ONE OF THE          -
CD                        FOLLOWING VALUES                                      -
CD                        0...NOEDITS                                           -
CD                        1...PRINT EDITS                                       -
CD                        2...WRITE EDITS TO AUXILIARY OUTPUT FILE              -
CD                        3...WRITE EDITS TO BOTH PRINT AND AUXILIARY           -
CD                            OUTPUT FILE                                       -
CD     NRCH(4)   *IEDTQ*  SEARCH QUANTITY EDIT OPTION                           -
CD                        TWO DIGIT NUMBER (IF) WHERE                           -
CD                                                                              -
CD                        I CONTROLS INTERMEDIATE PASS QUANTITY EDITS           -
CD                        F CONTROLS FINAL PASS QUANTITY EDITS                  -
CD                                                                              -
CD                        THE INTEGERS I AND F ARE ASSIGNED ONE OF THE          -
CD                        FOLLOWING VALUES                                      -
CD                        0...NOEDITS                                           -
CD                        1...PRINT EDITS                                       -
CD                        2...WRITE EDITS TO AUXILIARY OUTPUT FILE              -
CD                        3...WRITE EDITS TO BOTH PRINT AND AUXILIARY           -
CD                            OUTPUT FILE                                       -
CD     NRCH(5) *IBOUND*   SEARCH PARAMETER RANGE SENTINEL                       -
CD                        0...RANGE NOT EXCEEDED                                -
CD                        N...RANGE EXCEEDED N TIMES                            -
CD     NRCH(6) *IHIST(1)*PREVIOUS PASS-1 (N) AND METHOD (M) =10N+M              -
CD     NRCH(7) *IHIST(2)*PREVIOUS PASS (N) AND METHOD (M) =10N+M                -
CD     NRCH(8) *IHIST(3)*PRESENT PASS (N) AND METHOD (M)=10N+M                  -
CD     NRCH(9) *ICONV*    SEARCH TERMINATION SENTINEL                           -
CD                        0...INITIALIZED VALUE                                 -
CD                        1...SEARCH CONVERGED                                  -
CD                        2...SEARCH TERMINATED, MAXIMUM SEARCH PASSES          -
CD                            ACHIEVED                                          -
CD                        3...POOR CHOICE OF SEARCH PARAMETERS                  -
CD                        4...INSUFFICIENT TIME FOR NEXT SEARCH PASS            -
CD                        5...NEUTRONICS TERMINATED FOR INSUFFICIENT TIME-
CD                        6...RESTART, PREVIOUS TERMINATION CONDITION           -
CD                            UNKNOWN                                           -
CD     NRCH(10)           RESERVED
CD     SRCH1(1)*KEFF(1)*  PREVIOUS PASS-1 MULTIPLICATION FACTOR                 -
CD     SRCH1(2)*KEFF(2)*  PREVIOUS PASS MULTIPLICATION FACTOR                   -
CD     SRCH1(3)*KEFF(3)*  MOST RECENT MULTIPLICATION FACTOR                     -
CD     SRCH1(4)*DXNM2*    PREVIOUS PASS-1 DX                                    -
CD     SRCH1(5)*DXNM1*    PREVIOUS PASS DX                                      -
CD     SRCH1(6)*DXNTH*    MOST RECENT DX                                        -
CD     SRCH1(7)*DKNM2*    PREVIOUS PASS-1 K-EFFECTIVE CHANGE                    -
CD     SRCH1(8)*DKNM1*    PREVIOUS PASS K-EFFECTIVE CHANGE                      -
CD     SRCH1(9)*DKNTH*    MOST RECENT K-EFFECTIVE CHANGE                        -
C                                                                               -
C-------------------------------------------------------------------------------

C-------------------------------------------------------------------------------
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CR          COARSE MESH MODIFIERS FOR DIMENSION SEARCH                  -
CR                              (3D RECORD)                             -
C                                                                       -
CC          PRESENT IF ISRCH.EQ.5                                       -
C                                                                       -
CL    (SRHDI(I),I=1,NCINTI),(SRHDJ(J),J=1,NCINTJ),(SRHDK(K),K=1,NCINTK)-
C                                                                       -
CW    NCINTI+NCINTJ+NCINTK=NUMBER OF WORDS                              -
C                                                                       -
CD    SRHDI(I)          FIRST DIMENSION COARSE MESH MODIFIERS           -
CD    SRHDJ(J)          SECOND DIMENSION COARSE MESH MODIFIERS          -
CD    SRHDK(K)          THIRD DIMENSION COARSE MESH MODIFIERS           -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          NUCLIDES FOR PROPORTIONAL SEARCH AND SPECIAL SEARCH         -
CR                              (4D RECORD)                             -
C                                                                       -
CC          PRESENT IF ISRCH.EQ.7                                       -
C                                                                       -
CL    (NSHZ1(I),I=1,NSETS),(NSHZ2(I),I=1,NSETS),                        -
CL    ((HNNAMS(N,I),N=1,NISOSR),I=1,NSETS),(HNSHN(J),J=1,10)            -
C                                                                       -
CW    2*NSETS+MULT*(NISOSR*NSETS+10)=NUMBER OF WORDS                    -
C                                                                       -
CD    NSHZ1(I)          FIRST NUMBER OF A CONSECUTIVE SET OF ZONES     -
CD                          IF ISZOP.EQ.0, OR OF A CONSECUTIVE SET OF   -
CD                          SUBZONES IF ISZOP.EQ.1                      -
CD    NSHZ2(I)          LAST NUMBER OF A SET OF ZONES OR SUBZONES      -
CD    HNNAMS(N,I)       REFERENCE NAMES OF NUCLIDES WHOSE               -
CD                          CONCENTRATIONS ARE TO BE ADJUSTED           -
CD                          PROPORTIONATELY IN ABOVE ZONES (A6)         -
CD    HNSHN(J)  *N.A.*  SEARCH NUCLIDE REFERENCE USED AS NOTED BELOW    -
CD                          (A6)                                        -
C                                                                       -
CC                        HNNAMS CONCENTRATIONS ADJUSTED ACCORDING TO   -
CC                        C2 = C1*EI AND HNSHN CONCENTRATIONS ADJUSTED  -
CC                        ACCORDING TO C2 =C1 + C1*(1.0-EI)*CMOD WHERE  -
CC                          EI IS THE EIGENVALUE,                       -
CC                          C1 IS THE INITIAL CONCENTRATION, AND        -
CC                          C2 IS THE FINAL OR INTERMEDIATE VALUE OF    -
CC                             THE CONCENTRATION                        -
CC                                                                      -
CC              *MOD*     THE ANL SEARCH IMPLEMENTATION REQUIRES THAT   -
CC                        CONCENTRATIONS BE MODIFIED FOR ALL NUCLIDES   -
CC                        (NISOSR=NNS) PRESENT IN THE SUBZONES SPECIFIED-
CC                        ABOVE.  THESE ARE TERMED *MODIFIER* SUBZONES. -
CC                        DIRECT MODIFICATION OF ZONE NUCLIDES IS NOT   -
CC                        PERMITTED.  CONSEQUENTLY, NISOSR MUST EQUAL   -
CC                        NNS, THE MAXIMUM NUMBER OF NUCLIDES IN ANY    -
CC                        NUCLIDE SET, HENCE IN ANY SUBZONE. SUBZONE    -
CC                        TO ZONE ASSIGNMENTS ARE INDICATED IN THE NZSZ -
CC                        ARRAY GIVEN IN RECORD 3D OF DATA SET NDXSRF.  -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR  *N.A.* NUCLIDES FOR SEARCH INVOLVING WEIGHTED EIGENVALUE            -
CR              ADJUSTMENTS TO INITIAL CONCENTRATIONS                   -
CR                              (5D RECORD)                             -
C                                                                       -
CC          PRESENT IF ISRCH.EQ.9                                       -
C                                                                       -
CL    (NSHZ1(I),I=1,NSETS),(NSHZ2(I),I=1,NSETS),                        -
CL    ((HNNAMS(N,I),N=1,NISOSR),I=1,NSETS),                             -
CL    ((CHZDN(N,I),N=1,NISOSR),I=1,NSETS)                               -
C                                                                       -
CW    NSETS*(2+NISOSR*(1+MULT))=NUMBER OF WORDS                         -
C                                                                       -
CD    NSHZ1(I)          FIRST NUMBER OF A CONSECUTIVE SET OF ZONES     -
CD                          IF ISZOP.EQ.0, OR OF A CONSECUTIVE SET OF   -
CD                          SUBZONES IF ISZOP.EQ.1                      -
CD    NSHZ2(I)          LAST NUMBER OF A SET OF ZONES OR SUBZONES      -
CD    HNNAMS(N,I)       REFERENCE NAMES OF NUCLIDES WHOSE               -
CD                          CONCENTRATIONS ARE TO BE ADJUSTED (A6)      -
CD    CHZDN(N,I)        CONCENTRATION MODIFIERS                         -
C                                                                       -
CC                      CONCENTRATIONS ADJUSTED ACCORDING TO            -
CC                        C2 = C1+EI*CHZDN WHERE EI, C1, AND C2 ARE     -
CC                          AS DEFINED UNDER ISRCH .EQ. 7               -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR *NEW*    BUCKLING MODIFIERS FOR CRITICALITY SEARCH                   -
CR                              (6D RECORD)                             -
C                                                                       -
CC          PRESENT IF ISRCH.EQ.1                                       -
C                                                                       -
CL    (BKLMOD(I),I=1,NZONE)                                             -
C                                                                       -
CW    NZONE*MULT=NUMBER OF WORDS                                        -
C                                                                       -
CD    BKLMOD(I)         BUCKLING MODIFIER FOR ZONE I                    -
CD    NZONE             NRCH(2), THE NUMBER OF ZONES                    -
C                                                                       -
C-----------------------------------------------------------------------

CEOF                                                                    -
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C.8 ATFLUX

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C*****************************************************************************
C                       REVISED 11/30/76                                      -
C                                                                             -
CF          ATFLUX-IV                                                         -
CE          ADJOINT TOTAL FLUXES                                              -
C                                                                             -
C*****************************************************************************
CD                      ORDER OF GROUPS IS ACCORDING TO INCREASING
CD                      ENERGY.  NOTE THAT DOUBLE PRECISION
CD                      FLUXES ARE GIVEN WHEN MULT.EQ.2
C-----------------------------------------------------------------------------
CR          FILE IDENTIFICATION                                               -
C                                                                             -
CL     HNAME,(HUSE(I),I=1,2),IVERS                                            -
C                                                                             -
CW     1+3*MULT=NUMBER OF WORDS                                               -
C                                                                             -
CD     HNAME            HOLLERITH FILE NAME - ATFLUX - (A6)                   -
CD     HUSE(I)          HOLLERITH USER IDENTIFICATION (A6)                    -
CD     IVERS            FILE VERSION NUMBER                                   -
CD     MULT             DOUBLE PRECISION PARAMETER                            -
CD                          1- A6 WORD IS SINGLE WORD                          -
CD                          2- A6 WORD IS DOUBLE PRECISION WORD                -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          SPECIFICATIONS      (1D RECORD)                                   -
C                                                                             -
CL     NDIM,NGROUP,NINTI,NINTJ,NINTK,ITER,EFFK,ADUM,NBLOK                     -
C                                                                             -
CW     9 =NUMBER OF WORDS                                                     -
C                                                                             -
CD     NDIM             NUMBER OF DIMENSIONS                                  -
CD     NGROUP           NUMBER OF ENERGY GROUPS                               -
CD     NINTI            NUMBER OF FIRST DIMENSION FINE MESH INTERVALS         -
CD     NINTJ            NUMBER OF SECOND DIMENSION FINE MESH INTERVALS        -
CD     NINTK            NUMBER OF THIRD DIMENSION FINE MESH INTERVALS.        -
CD                      NINTK.EQ.1 IF NDIM.LE.2                               -
CD     ITER             OUTER ITERATION NUMBER AT WHICH FLUX WAS              -
CD                      WRITTEN                                               -
CD     EFFK             EFFECTIVE MULTIPLICATION FACTOR                       -
CD     ADUM             RESERVED                                              -
CD     NBLOK            DATA BLOCKING FACTOR                                  -
CD                         IF NDIM.EQ.1 THE GROUP VARIABLE IS BLOCKED         -
CD                            INTO NBLOK BLOCKS (SEE 2D RECORD BELOW)         -
CD                         IF NDIM.GE.2 THE 2ND DIMENSION VARIABLE IS         -
CD                            BLOCKED INTO NBLOK BLOCKS (SEE 3D RECORD)       -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          ONE DIMENSIONAL ADJOINT TOTAL FLUX   (2D RECORD)                  -
C                                                                             -
CC          PRESENT IF NDIM.EQ.1                                              -
C                                                                             -
CL     ((FADJ(I,J),I=1,NINTI),J=JL,JU)-----SEE STRUCTURE BELOW-----           -
C                                                                             -
CW     NINTI*(JU - JL + 1)*MULT = NUMBER OF WORDS                             -
C                                                                             -
C      DO 1 M=1,NBLOK                                                         -
C    1 READ(N)   *LIST AS ABOVE*                                              -
C                                                                             -
CC          WITH M AS THE BLOCK INDEX, JL=(M-1)*((NGROUP-1)/NBLOK+1)+1        -
CC          AND JU=MINO(NGROUP,JUP) WHERE JUP=M*((NGROUP-1)/NBLOK+1)          -
C                                                                             -
CD     FADJ(I,J)           ONE DIMENSIONAL ADJOINT TOTAL FLUX BY INTERVAL    -
CD                         AND GROUP.                                         -
C                                                                             -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          MULTI-DIMENSIONAL ADJOINT TOTAL FLUX   (3D RECORD)                -
C                                                                             -
CC          PRESENT IF NDIM.GE.2                                              -
C                                                                             -
CL     ((FADJ(I,J),I=1,NINTI)J=JL,JU)-----SEE STRUCTURE BELOW-----            -
C                                                                             -
CW     NINTI*(JU - JL + 1)*MULT = NUMBER OF WORDS                             -
C                                                                             -
C      DO 1 L=1,NGROUP                                                        -
C      DO 1 K=1,NINTK                                                         -
C      DO 1 M=1,NBLOK                                                         -
C    1 READ(N)   *LIST AS ABOVE*                                              -
C                                                                             -
CC          WITH M AS THE BLOCK INDEX, JL=(M-1)*((NINTJ-1)/NBLOK +1)+1        -
CC          AND JU=MINO(NINTJ,JUP) WHERE JUP=M*((NINTJ-1)/NBLOK +1)           -
C                                                                             -
CD     FADJ(I,J)           MULTI-DIMENSIONAL ADJOINT TOTAL FLUX              -
CD                         BY INTERVAL AND GROUP.                             -
C                                                                             -
C-----------------------------------------------------------------------------
CEOF
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C.9 RZFLUX

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C*****************************************************************************
C                        REVISED 11/30/76                                     -
C                                                                             -
CF          RZFLUX-IV                                                         -
C                                                                             -
CE          REGULAR ZONE FLUX BY GROUP, AVERAGED OVER EACH ZONE               -
C                                                                             -
C*****************************************************************************
C-----------------------------------------------------------------------------
CR          FILE IDENTIFICATION                                               -
C                                                                             -
CL     HNAME,(HUSE(I),I=1,2),IVERS                                            -
C                                                                             -
CW     1+3*MULT=NUMBER OF WORDS                                               -
C                                                                             -
CD     HNAME              HOLLERITH FILE NAME - RZFLUX - (A6)                 -
CD     HUSE(I)            HOLLERITH USER IDENTIFICATION (A6)                  -
CD     IVERS              FILE VERSION NUMBER                                 -
CD     MULT               DOUBLE PRECISION PARAMETER                          -
CD                           1- A6 WORD IS SINGLE WORD                         -
CD                           2- A6 WORD IS DOUBLE PRECISION WORD               -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          SPECIFICATIONS      (1D RECORD)                                   -
C                                                                             -
CL     TIME,POWER,VOL,EFFK,EIVS,DKDS,TNL,TNA,TNSL,TNBL,TNBAL,TNCRA,           -
CL    1(X(I),I=1,3),NBLOK,ITPS,NZONE,NGROUP,NCY                              -
C                                                                             -
CW     20=NUMBER OF WORDS                                                     -
C                                                                             -
CD     TIME               REFERENCE REAL TIME, DAYS                          -
CD     POWER              POWER LEVEL FOR ACTUAL NEUTRONICS PROBLEM,WATTS-   -
CD                          THERMAL                                           -
CD     VOL                VOLUME OVER WHICH POWER WAS DETERMINED, CC         -
CD     EFFK               MULTIPLICATION FACTOR                              -
CD     EIVS               EIGENVALUE OF SEARCH OF SEARCH PROBLEM             -
CD     DKDS               DERIVATIVE OF SEARCH PROBLEM                       -
CD     TNL                TOTAL NEUTRON LOSSES                               -
CD     TNA                TOTAL NEUTRON ABSORPTIONS                          -
CD     TNSL               TOTAL NEUTRON SURFACE LEAKAGE                      -
CD     TNBL               TOTAL NEUTRON BUCKLING LOSS                        -
CD     TNBAL              TOTAL NEUTRON BLACK ABSORBER LOSS                  -
CD     TNCRA              TOTAL NEUTRON CONTROL ROD ABSORPTIONS              -
CD     X(I),I=1,3         RESERVED                                           -
CD     NBLOK              DATA BLOCKING FACTOR.  THE GEOMETRIC ZONE          -
CD                          VARIABLE IS BLOCKED INTO NBLOK BLOCKS.           -
CD     ITPS               ITERATIVE PROCESS STATE                            -
CD                           =0, NO ITERATIONS DONE                           -
CD                           =1, CONVERGENCE SATISFIED                        -
CD                           =2, NOT CONVERGED, BUT CONVERGING                -
CD                           =3, NOT CONVERGED, NOT CONVERGING                -
CD     NZONE              NUMBER OF GEOMETRIC ZONES                          -
CD     NGROUP             NUMBER OF NEUTRON ENERGY GROUPS                    -
CD     NCY                REFERENCE COUNT (CYCLE NUMBER)                     -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          FLUX VALUES       (2D RECORD)                                     -
C                                                                             -
CL     ((ZGF(K,J),K=1,NGROUP),J=JL,JU) -----SEE STRUCTURE BELOW-----          -
C                                                                             -
CW     NGROUP*(JU-JL+1) = NUMBER OF WORDS                                     -
C                                                                             -
C      DO 1 M=1,NBLOK                                                         -
C    1 READ(N)   *LIST AS ABOVE*                                              -
C                                                                             -
CC          WITH M AS THE BLOCK INDEX, JL=(M-1)*((NZONE-1)/NBLOK +1)+1       -
CC          AND JU=MIN0(NZONE,JUP) WHERE JUP=M*((NZONE-1)/NBLOK +1)          -
C                                                                             -
CD     ZGF(K,J)           REGULAR ZONE FLUX BY GROUP, AVERAGED OVER ZONE     -
CD                        NEUTRONS/SEC-CM**2                                 -
C                                                                             -
C-----------------------------------------------------------------------------
CEOF
```

C.10 PWDINT

```
C*****************************************************************************
C                        REVISED 11/30/76                                     -
C                                                                             -
CF          PWDINT-IV                                                         -
C                                                                             -
CE          POWER DENSITY BY INTERVAL                                         -
C                                                                             -
C*****************************************************************************
C-----------------------------------------------------------------------------
CR          FILE IDENTIFICATION                                               -
C                                                                             -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                             -
C                                                                             -
CW    1+3*MULT=NUMBER OF WORDS                                                -
C                                                                             -
CD    HNAME             HOLLERITH FILE NAME - PWDINT - (A6)                   -
CD    HUSE(I)           HOLLERITH USER IDENTIFICATION (A6)                    -
CD    IVERS             FILE VERSION NUMBER                                   -
CD    MULT              DOUBLE PRECISION PARAMETER                            -
CD                          1- A6 WORD IS SINGLE WORD                         -
CD                          2- A6 WORD IS DOUBLE PRECISION WORD               -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR          SPECIFICATIONS     (1D RECORD)                                    -
C                                                                             -
CL    TIME, POWER, VOL, NINTI,NINTJ,NINTK,NCY,NBLOK                           -
C                                                                             -
CW    8=NUMBER OF WORDS                                                       -
C                                                                             -
CD    TIME              REFERENCE REAL TIME, DAYS                             -
CD    POWER             POWER LEVEL FOR ACTUAL NEUTRONICS PROBLEM,            -
CD                          WATTS THERMAL                                     -
CD    VOL               VOLUME OVER WHICH POWER WAS DETERMINED,CC             -
CD    NINTI             NUMBER OF FIRST DIMENSION FINE INTERVALS              -
CD    NINTJ             NUMBER OF SECOND DIMENSION FINE INTERVALS             -
CD    NINTK             NUMBER OF THIRD DIMENSION FINE INTERVALS              -
CD    NCY               REFERENCE COUNT (CYCLE NUMBER)                        -
CD    NBLOK             DATA BLOCKING FACTOR. THE SECOND DIMENSION            -
CD                         VARIABLE IS BLOCKED INTO NBLOK BLOCKS.             -
C                                                                             -
C-----------------------------------------------------------------------------
C-----------------------------------------------------------------------------
CR                      POWER DENSITY VALUES   (2D RECORD)                    -
C                                                                             -
CL    ((PWR(I,J), I=1,NINTI),J=JL,JU)-----SEE STRUCTURE BELOW-----            -
C                                                                             -
CW    NINTI*(JU - JL + 1) = NUMBER OF WORDS                                   -
C                                                                             -
CS    DO 1 K=1,KM                                                             -
CS    DO 1 M=1,NBLOK                                                          -
CS  1 READ(N) *LIST AS ABOVE*                                                 -
C                                                                             -
CC          WITH M AS THE BLOCK INDEX, JL=(M-1)*((NINTJ-1)/NBLOK +1)+1        -
CC          AND JU=MINO(NINTJ,JUP) WHERE JUP=M*((NINTJ-1)/NBLOK +1)           -
C                                                                             -
CD    PWR(I,J)          POWER DENSITY BY INTERVAL, WATTS/CC                   -
C                                                                             -
C-----------------------------------------------------------------------------
CEOF
```

Appendix D

DIF3D CODE-DEPENDENT BINARY INTERFACE FILE DESCRIPTIONS

D.1 COMPXS

```
C*****************************************************************************
C                                                                             -
C                       PREPARED 3/7/78 AT ANL                                -
C                       LAST REVISED 12/5/80                                  -
C                                                                             -
CF          COMPXS                                                            -
CE          MACROSCOPIC COMPOSITION CROSS SECTIONS                            -
C                                                                             -
C*****************************************************************************


C-----------------------------------------------------------------------------
CS          FILE STRUCTURE                                                    -
CS                                                                            -
CS          RECORD TYPE                          PRESENT IF                   -
CS          ===================================  =========================-
CS          SPECIFICATIONS                       ALWAYS                       -
CS          COMPOSITION INDEPENDENT DATA         ALWAYS                       -
CS     ********* (REPEAT FOR ALL COMPOSITIONS)                                -
CS     *    COMPOSITION SPECIFICATIONS           ALWAYS                       -
CS     *  ****** (REPEAT FOR ALL ENERGY GROUPS                                -
CS     *  *       IN THE ORDER OF DECREASING                                  -
CS     *  *       ENERGY)                                                     -
CS     *  *  COMPOSITION MACROSCOPIC GROUP     ALWAYS                       -
CS     *  *  CROSS SECTIONS                                                   -
CS     *********                                                             -
CS          FISSION POWER CONVERSION FACTORS     ALWAYS                       -
CS                                                                            -
C                                                                             -
C-----------------------------------------------------------------------------


CD     NGROUP            NUMBER OF ENERGY GROUPS.
CD     ICHI              PROMPT FISSION SPECTRUM FLAG FOR THIS
CD                       COMPOSITION. ICHI=-1 IF COMPOSITION USES THE
CD                       SET-WIDE PROMPT CHI GIVEN IN SET CHI RECORD
CD                       (BELOW). ICHI=0 IF COMPOSITION IS NOT
CD                       FISSIONABLE. ICHI=1 FOR COMPOSITION PROMPT CHI
CD                       VECTOR. ICHI=NGROUP FOR COMPOSITION PROMPT CHI
CD                       MATRIX.
CD     NUP(I)            NUMBER OF GROUPS OF UPSCATTERING INTO GROUP I
CD                       FROM LOWER ENERGY GROUPS FOR THE CURRENT
CD                       COMPOSITION
CD     NDN(I)            NUMBER OF GROUPS OF DOWNSCATTERING INTO GROUP I
CD                       FROM HIGHER ENERGY GROUPS FOR THE CURRENT
CD                       COMPOSITION
CD     ISCHI             PROMPT FISSION SPECTRUM FLAG. ISCHI=0 IF
CD                       THERE IS NO SET-WIDE PROMPT CHI. ISCHI=1 IF
CD                       THERE IS A SET-WIDE PROMPT CHI VECTOR.
CD                       ISCHI=NGROUP IF THERE IS A SET-WIDE PROMPT
CD                       CHI MATRIX.
CD     NFAM              NUMBER OF DELAYED NEUTRON FAMILIES.
CD     MULT              2 FOR IBM MACHINES, 1 OTHERWISE.


C-----------------------------------------------------------------------------
CR          SPECIFICATIONS (TYPE 1)                                           -
C                                                                             -
CL     NCMP,NGROUP,ISCHI,NFCMP,MAXUP,MAXDN,NFAM,NDUM1,NDUM2,NDUM3             -
C                                                                             -
CW     10                                                                     -
C                                                                             -
CD     NCMP              NUMBER OF COMPOSITIONS.                             -
CD     NFCMP             NUMBER OF FISSIONABLE COMPOSITIONS.                 -
CD     MAXUP             MAXIMUM NUMBER OF GROUPS OF UPSCATTERING FOR        -
CD                       THE SET.                                            -
CD     MAXDN             MAXIMUM NUMBER OF GROUPS OF DOWNSCATTERING          -
CD                       FOR THE SET.                                        -
CD     NDUM1             RESERVED.                                           -
CD     NDUM2             RESERVED.                                           -
CD     NDUM3             RESERVED.                                           -
C                                                                             -
C-----------------------------------------------------------------------------


C-----------------------------------------------------------------------------
CR          COMPOSITION INDEPENDENT DATA (TYPE 2)                             -
C                                                                             -
CC          ALWAYS PRESENT                                                    -
C                                                                             -
CL     ((CHI(I,J),I=1,ISCHI),J=1,NGROUP),(VEL(J),J=1,NGROUP),                 -
CL    1(EMAX(J),J=1,NGROUP),EMIN,((CHID(J,K),J=1,NGROUP),K=1,NFAM),           -
CL    2(FLAM(K),K=1,NFAM),(NKFAM(J),J=1,NCMP)                                 -
C                                                                             -
CW     MULT*(NGROUP*(ISCHI+2+NFAM)+1+NFAM)+NCMP                               -
C                                                                             -
CD     CHI               PROMPT FISSION FRACTION INTO GROUP J FROM           -
CD                       GROUP I. IF ISCHI=1, THE LIST REDUCES TO            -
CD                       (CHI(J),J=1,NGROUP), WHERE CHI(J) IS THE            -
CD                       FISSION FRACTION INTO GROUP J.                      -
CD     VEL               MEAN NEUTRON VELOCITY IN GROUP J (CM/SEC).          -
CD     EMAX              MAXIMUM ENERGY BOUND OF GROUP J (EV).               -
CD     EMIN              MINIMUM ENERGY BOUND OF SET (EV).                   -
CD     CHID              FRACTION OF DELAYED NEUTRONS EMITTED INTO           -
CD                       NEUTRON ENERGY GROUP J FROM PRECURSOR               -
```

```
CD                  FAMILY K.                                          -
CD    FLAM          DELAYED NEUTRON PRECURSOR DECAY CONSTANT           -
CD                  FOR FAMILY K.                                      -
CD    NKFAM         NUMBER OF FAMILIES TO WHICH FISSION IN             -
CD                  COMPOSITION J CONTRIBUTES DELAYED NEUTRON          -
CD                  PRECURSORS.                                        -
C                                                                      -
C----------------------------------------------------------------------
```

```
C----------------------------------------------------------------------
CR          COMPOSITION SPECIFICATIONS (TYPE 3)                        -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    ICHI,(NUP(I),I=1,NGROUP),(NDN(I),I=1,NGROUP),                    -
CL   1(NUMFAM(I),I=1,NKFAMI)                                           -
C                                                                      -
CC    NKFAMI = NKFAM(K)                                                -
C                                                                      -
CW    1+2*NGROUP+NKFAMI                                                -
C                                                                      -
CD    NUMFAM        FAMILY NUMBER OF THE I-TH YIELD VECTOR IN          -
CD                  ARRAY SNUDEL(I).                                   -
C                                                                      -
C----------------------------------------------------------------------
```

```
C----------------------------------------------------------------------
CR          COMPOSITION MACROSCOPIC GROUP CROSS SECTIONS (TYPE 4)      -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    XA,XTOT,XREM,XTR,XF,XNF,(CHI(I),I=1,ICHI),                       -
CL   1(XSCATU(I),I=1,NUMUP),XSCATJ,(XSCATD(I),I=1,NUMDN),              -
CL   2PC,A1,B1,A2,B2,A3,B3,(SNUDEL(I),I=1,NKFAMI),XN2N                 -
C                                                                      -
CC    NUMUP = NUP FOR THE CURRENT GROUP                                -
CC    NUMDN = NDN FOR THE CURRENT GROUP                                -
CC    NKFAMI = NKFAM(K)                                                -
C                                                                      -
CW    MULT*(15+ICHI+NUMUP+NUMDN+NKFAMI)   IF ICHI.GT.0                 -
CW    MULT*(15+NUMUP+NUMDN+NKFAMI)        IF ICHI.EQ.-1                -
CW    MULT*(13+NUMUP+NUMDN+NKFAMI)        IF ICHI.EQ.0                 -
C                                                                      -
CD    XA            ABSORPTION CROSS SECTION.                        -
CD    XTOT          TOTAL CROSS SECTION.                             -
CD    XREM          REMOVAL CROSS SECTION, TOTAL CROSS SECTION       -
CD                  FOR REMOVING A NEUTRON FROM GROUP J DUE TO ALL   -
CD                  PROCESSES.                                       -
CD    XTR           TRANSPORT CROSS SECTION.                         -
CD    XF            FISSION CROSS SECTION, PRESENT ONLY IF           -
CD                  ICHI.NE.0.                                       -
CD    XNF           TOTAL NUMBER OF NEUTRONS EMITTED PER FISSION     -
CD                  TIMES XF, PRESENT ONLY IF ICHI.NE.0.             -
CD    CHI           PROMPT FISSION FRACTION INTO GROUP J FROM        -
CD                  GROUP I, PRESENT ONLY IF ICHI.GT.0. IF ICHI=1,   -
CD                  THE LIST REDUCES TO THE SINGLE NUMBER CHI,       -
CD                  WHICH IS THE PROMPT FISSION FRACTION INTO        -
CD                  GROUP J.                                         -
CD    XSCATU        TOTAL SCATTERING CROSS SECTION INTO GROUP J      -
CD                  FROM GROUPS J+NUP(J),J+NUP(J)-1,...,J+2,J+1,     -
CD                  PRESENT ONLY IF NUP(J).GT.0.                     -
CD    XSCATJ        TOTAL SELF-SCATTERING CROSS SECTION FROM         -
CD                  GROUP J TO GROUP J.                              -
CD    XSCATD        TOTAL SCATTERING CROSS SECTION INTO GROUP J      -
CD                  FROM GROUPS J-1,J-2,...,J-NDN(J), PRESENT        -
CD                  ONLY IF NDN(J).GT.0.                             -
CD    PC            PC TIMES THE GROUP J REGION INTEGRATED           -
CD                  FLUX FOR THE REGIONS CONTAINING THE CURRENT      -
CD                  COMPOSITION YIELDS THE POWER IN WATTS IN THOSE   -
CD                  REGIONS AND ENERGY GROUP J DUE TO FISSIONS       -
CD                  AND NON-FISSION ABSORPTIONS.                     -
CD    A1            FIRST DIMENSION DIRECTIONAL DIFFUSION            -
CD                  COEFFICIENT MULTIPLIER.                          -
CD    B1            FIRST DIMENSION DIRECTIONAL DIFFUSION            -
CD                  COEFFICIENT ADDITIVE TERM.                       -
CD    A2            SECOND DIMENSION DIRECTIONAL DIFFUSION           -
CD                  COEFFICIENT MULTIPLIER.                          -
CD    B2            SECOND DIMENSION DIRECTIONAL DIFFUSION           -
CD                  COEFFICIENT ADDITIVE TERM.                       -
CD    A3            THIRD DIMENSION DIRECTIONAL DIFFUSION            -
CD                  COEFFICIENT MULTIPLIER.                          -
CD    B3            THIRD DIMENSION DIRECTIONAL DIFFUSION            -
CD                  COEFFICIENT ADDITIVE TERM.                       -
CD    SNUDEL        NUMBER OF DELAYED NEUTRON PRECURSORS PRODUCED     -
CD                  IN FAMILY NUMBER NUMFAM(I) PER FISSION           -
CD                  IN GROUP J.                                      -
CD    XN2N          N,2N REACTION CROSS SECTION                      -
C                                                                      -
CN                  THE MACROSCOPIC XN2N(J) TIMES THE FLUX IN GROUP-
CN                  J GIVES THE RATE AT WHICH N,2N REACTIONS OCCUR   -
CN                  IN GROUP J.  THUS, FOR N,2N SCATTERING,          -
CN                  XN2N(J)=0.5*(SUM OF SCAT(J TO G)) SUMMED OVER    -
CN                  ALL G WHERE SCAT IS THE N,2N SCATTERING MATRIX.  -
C
C----------------------------------------------------------------------
```

```
C----------------------------------------------------------------------
CR          FISSION POWER CONVERSION FACTORS (TYPE 5)                  -
C                                                                      -
CC          ALWAYS PRESENT                                             -
C                                                                      -
CL    (FPWS(I),I=1,NCMP)                                               -
C                                                                      -
CW    MULT*NCMP                                                        -
C                                                                      -
```

```
CD    FPWS              FISSIONS/WATT-SECOND FOR EACH COMPOSITION      -
C                                                                      -
C----------------------------------------------------------------------

CEOF
```

D.2 DIF3D

```
C**********************************************************************
C                       REVISED 5/26/83                                -
C                                                                      -
CF          DIF3D                                                      -
CE          ONE-, TWO-, AND THREE-DIMENSIONAL DIFFUSION THEORY         -
CE          MODULE DEPENDENT BINARY INPUT                              -
C                                                                      -
C**********************************************************************


C----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
CD    HNAME             HOLLERITH FILE NAME - DIF3D - (A6)             -
CD    HUSE(I)           HOLLERITH USER IDENTIFICATION (A6)             -
CD    IVERS             FILE VERSION NUMBER                            -
CD    MULT              DOUBLE PRECISION PARAMETER                     -
CD                          1- A6 WORD IS SINGLE WORD                  -
CD                          2- A6 WORD IS DOUBLE PRECISION WORD        -
C                                                                      -
C----------------------------------------------------------------------


C----------------------------------------------------------------------
CR          PROBLEM TITLE, STORAGE AND DUMP SPECIFICATIONS (1D RECORD) -
C                                                                      -
CL    (TITLE(I),I=1,11),MAXSIZ,MAXBLK,IPRINT                           -
C                                                                      -
CW    3+11*MULT=NUMBER OF WORDS                                        -
C                                                                      -
CD    TITLE             ANY ALPHANUMERIC CHARACTERS                    -
CD    MAXSIZ            POINTR CONTAINER ARRAY SIZE IN FAST CORE       -
CD                      MEMORY (FCM) IN REAL*8 WORDS                   -
CD    MAXBLK            POINTR CONTAINER ARRAY SIZE IN EXTENDED CORE   -
CD                      MEMORY (ECM) IN REAL*8 WORDS                   -
CD    IPRINT            POINTER DEBUGGING EDIT                         -
CD                      0...NO DEBUGGING PRINTOUT                      -
CD                      1...DEBUGGING DUMP PRINTOUT                    -
CD                      2...DEBUGGING TRACE PRINTOUT                   -
CD                      3...BOTH DUMP AND TRACE PRINTOUT               -
C                                                                      -
C----------------------------------------------------------------------


C----------------------------------------------------------------------
CR          PROBLEM INTEGER CONTROL PARAMETERS (2D RECORD)             -
C                                                                      -
CL    IPROBT,ISOLNT,IXTRAP,MINBSZ,NOUTMX,IRSTRT,LIMTIM,NUPMAX,IOSAVE,  -
CL    1IOMEG,INRMAX,NUMORP,IRETRN,(IEDF(I),I=1,10),NOUTBQ,IOFLUX,      -
CL    2NOEDIT,NOD3ED,ISRHED,NSN,NSWMAX,IAPRX,IAPRXZ,NCMI,ISEXTR,NZSWP, -
CL    3NCMRZS,(IDUM(I),I=1,9)                                          -
C                                                                      -
CW    45=NUMBER OF WORDS                                               -
C                                                                      -
CD    IPROBT            PROBLEM TYPE                                   -
CD                      0...K-EFFECTIVE PROBLEM                        -
CD                      1...FIXED SOURCE PROBLEM                       -
CD    ISOLNT            SOLUTION TYPE                                  -
CD                      0...REAL SOLUTION                              -
CD                      1...ADJOINT SOLUTION                           -
CD                      2...BOTH REAL AND ADJOINT SOLUTION             -
CD    IXTRAP            CHEBYSHEV ACCELERATION OF OUTER ITERATIONS     -
CD                      0...YES, ACCELERATE THE OUTER ITERATIONS       -
CD                      1...NO ACCELERATION                            -
CD    MINBSZ            MINIMUM PLANE-BLOCK (RECORD) SIZE IN REAL*8    -
CD                      WORDS FOR I/O TRANSFERS IN THE CONCURRENT      -
CD                      ITERATION STRATEGY                             -
CD    NOUTMX            OUTER ITERATION CONTROL                        -
CD                     -3...BYPASS DIF3D MODULE.                       -
CD                     -2...PERFORM NEUTRONICS EDITS ONLY              -
CD                     -1...PERFORM NEUTRONICS EDITS AND CALCULATE     -
CD                         OPTIMUM OVERRELAXATION FACTORS ONLY         -
CD                   .GE.0...MAXIMUM NUMBER OF OUTER ITERATIONS        -
CD    IRSTRT            RESTART FLAG                                   -
CD                      0...THIS IS NOT A RESTART                      -
CD                      1...THIS IS A RESTART                          -
CD    LIMTIM            JOB TIME LIMIT, MAXIMUM (CP AND PP (OR WAIT))  -
CD                      PROCESSOR SECONDS                              -
CD    NUPMAX            NUMBER OF UPSCATTER ITERATIONS                 -
CD                      PER OUTER ITERATION                            -
CD    IOSAVE            CONCURRENT ITERATION EFFICIENCY OPTION         -
CD                      0...PERFORM THE ESTIMATED NO. OF INNER         -
CD                         ITERATIONS FOR EACH GROUP                   -
CD                      1...AVOID THE LAST PASS OF INNER ITERATIONS     -
CD                         IN THOSE GROUPS FOR WHICH THE NUMBER OF     -
CD                         INNER ITERATIONS IN THE LAST PASS ARE LESS  -
CD                         THAN A CODE DEPENDENT THRESHOLD             -
CD    IOMEG             OPTIMUM OVERRELAXATION FACTOR ESTIMATION       -
CD                      ACCELERATION OPTION.                           -
CD                      0...NO ACCELERATION.                           -
CD                      1...ASYMPTOTIC EXTRAPOLATION OF ITERATIONS IN  -
CD                         THE OPTIMUM OVERRELAXATION FACTOR           -
CD                         CALCULATION.                                -
CD    INRMAX            MAXIMUM NUMBER OF ITERATIONS PERMITTED DURING  -
```

```
CD                THE OPTIMUM OVERRELAXATION FACTOR ESTIMATION  -
CD                PROCESS FOR EACH INNER (WITHIN GROUP)         -
CD                ITERATION MATRIX.                             -
CD   NUMORP       NUMBER OF OPTIMUM OVERRELAXATION FACTORS      -
CD   IRETRN       FLAG INDICATING CAUSE OF OUTER ITERATION      -
CD                TERMINATION                                   -
CD                0...INITIAL VALUE, PRIOR TO OUTER ITERATIONS  -
CD                1...OUTER ITERATIONS CONVERGED                -
CD                2...MAXIMUM NUMBER OF OUTER ITERATIONS        -
CD                    PERFORMED                                 -
CD                3...TIME LIMIT                                -
CD   IEDF(1)      PROBLEM DESCRIPTION EDIT (IN ADDITION TO USER -
CD                INPUT SPECIFICATIONS WHICH ARE ALWAYS EDITED  -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(2)      GEOMETRY (REGION TO MESH INTERVAL) MAP EDIT   -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(3)      GEOMETRY (ZONE TO MESH INTERVAL) MAP EDIT     -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(4)      MACROSCOPIC CROSS SECTION EDIT                -
CD                ENTER TWO DIGIT NUMBER SP WHERE               -
CD                                                              -
CD                S CONTROLS THE SCATTERING CROSS SECTIONS EDIT -
CD                P CONTROLS THE PRINCIPAL CROSS SECTIONS EDIT  -
CD                                                              -
CD                THE INTEGERS S AND P SHOULD BE ASSIGNED ONE OF -
CD                THE FOLLOWING VALUES (LEADING ZEROES ARE      -
CD                IRRELEVANT)                                   -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(5)      BALANCE EDITS                                 -
CD                ENTER 3 DIGIT NUMBER GBR WHERE                -
CD                                                              -
CD                G CONTROLS GROUP BALANCE EDITS INTEGRATED OVER -
CD                  THE REACTOR                                 -
CD                B CONTROLS REGION BALANCE EDIT BY GROUP       -
CD                R CONTROLS REGION BALANCE EDIT TOTALS         -
CD                  (INCLUDING NET PRODUCTION AND ENERGY MEDIANS)-
CD                                                              -
CD                THE INTEGERS G, B, AND R SHOULD BE ASSIGNED   -
CD                ONE OF THE FOLLOWING VALUES (LEADING ZEROES   -
CD                ARE IRRELEVANT)                               -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILES                              -
CD   IEDF(6)      POWER EDITS                                   -
CD                ENTER 2 DIGIT NUMBER RM WHERE                 -
CD                                                              -
CD                R CONTROLS REGION POWER AND AVERAGE POWER     -
CD                  EDITS                                       -
CD                M CONTROLS POWER DENSITY BY MESH INTERVAL     -
CD                  EDIT (PWDINT)                               -
CD                                                              -
CD                THE INTEGERS R AND M SHOULD BE ASSIGNED ONE OF -
CD                THE FOLLOWING VALUES (LEADING ZEROES ARE      -
CD                IRRELEVANT)                                   -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(7)      TOTAL FLUX EDITS                              -
CD                ENTER 3 DIGIT INTEGER RMB WHERE               -
CD                                                              -
CD                R CONTROLS TOTAL FLUX EDIT BY REGION AND GROUP -
CD                  INCLUDING GROUP AND REGION TOTALS           -
CD                M CONTROLS TOTAL FLUX EDIT BY MESH INTERVAL   -
CD                  INTEGRATED OVER GROUP                       -
CD                B CONTROLS TOTAL FLUX EDIT BY MESH INTERVAL   -
CD                  AND GROUP (RTFLUX OR ATFLUX)                -
CD                                                              -
CD                THE INTEGERS R, M, AND B SHOULD BE ASSIGNED   -
CD                ONE OF THE FOLLOWING VALUES (LEADING ZEROES   -
CD                ARE IRRELEVANT)                               -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(8)      ZONE AVERAGED FLUX EDIT                       -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(9)      REGION AVERAGED FLUX EDIT                     -
CD                0...NO EDITS                                  -
CD                1...PRINT EDITS                               -
CD                2...WRITE EDITS TO AUXILIARY OUTPUT FILE      -
CD                3...WRITE EDITS TO BOTH PRINT AND AUXILIARY   -
CD                    OUTPUT FILE                               -
CD   IEDF(10)     STANDARD INTERFACE FILES TO BE WRITTEN IN      -
```

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CD                ADDITION TO RTFLUX AND/OR ATFLUX                -
CD                0...NONE                                        -
CD                1...WRITE PWDINT                                -
CD                2...WRITE RZFLUX                                -
CD                3...WRITE BOTH PWDINT AND RZFLUX                -
CD   NOUTBQ       NUMBER OF OUTER (POWER) ITERATIONS BEFORE        -
CD                ASYMPTOTIC EXTRAPOLATION OF NEAR CRITICAL       -
CD                SOURCE PROBLEM.                                 -
CD   IOFLUX       FLAT FLUX GUESS SENTINEL.                       -
CD                0...FLAT FLUX GUESS = 1.0                       -
CD                1...FLAT FLUX GUESS = 0.0                       -
CD   NOEDIT       PRINT FILE MASTER CONTROL FLAG                  -
CD                0...PRINT GENERAL RUN INFORMATION AND           -
CD                    REQUESTED EDITS                             -
CD                1...SUPPRESS ALL OUTPUT EXCEPT DIAGNOSTIC       -
CD                    EDITS AND THE ITERATION HISTORY             -
CD                2...SUPPRESS ALL OUTPUT EXCEPT DIAGNOSTIC EDITS
CD   NOD3ED       D3EDIT FILE MASTER CONTROL FLAG                 -
CD                0...WRITE REQUESTED EDITS ON D3EDIT FILE        -
CD                1...DO NOT WRITE D3EDIT FILE                    -
CD   ISRHED       MASTER NEUTRONICS EDIT SENTINEL DURING          -
CD                CRITICALITY SEARCHES ONLY.                      -
CD               -1...SUPPRESS ALL DIF3D EDITS EXCEPT ITERATION   -
CD                    HISTORY AND ERROR DIAGNOSTICS.              -
CD                0...EDIT INPUT DATA ON 1ST SEARCH PASS, OUTPUT  -
CD                    FLUX INTEGRALS UPON CONVERGENCE OR UPON     -
CD                    ACHIEVING THE MAXIMUM SEARCH PASS LIMIT.    -
CD                N...ALSO EDIT SPECIFIED DIF3D EDITS EVERY N-TH  -
CD                    SEARCH PASS.                                -
CD   NSN          SN ORDER (TRANSPORT OPTION)                     -
CD   NSWMAX       MAXIMUM ALLOWED NUMBER OF LINE SWEEPS PER LINE  -
CD                PER INNER ITERATION (TRANSPORT OPTION).         -
CD   IAPRX        ORDER OF NODAL APPROXIMATION IN HEX-PLANE        -
CD                (NODAL HEXAGONAL GEOMETRY OPTION)               -
CD                2...NH2 APPROXIMATION                           -
CD                3...NH3 APPROXIMATION                           -
CD                4...NH4 APPROXIMATION                           -
CD   IAPRXZ       ORDER OF NODAL APPROXIMATION IN Z-DIRECTION      -
CD                (NODAL HEXAGONAL GEOMETRY OPTION)               -
CD                2...QUADRATIC APPROXIMATION                     -
CD                3...CUBIC APPROXIMATION                         -
CD   NCMI         COARSE-MESH REBALANCE ACCELERATION CONTROL       -
CD                (NODAL HEXAGONAL GEOMETRY OPTION)               -
CD               -1...NO COARSE-MESH REBALANCE ACCELERATION        -
CD              .GE.0...NUMBER OF COARSE-MESH REBALANCE ITERATIONS -
CD                    PER OUTER ITERATION                         -
CD   ISEXTR       ASYMPTOTIC SOURCE EXTRAPOLATION OF OUTER         -
CD                ITERATIONS (NODAL HEXAGONAL GEOMETRY OPTION)    -
CD                0...APPLY ASYMPTOTIC SOURCE EXTRAPOLATION TO    -
CD                    OUTER ITERATIONS                            -
CD                1...NO ASYMPTOTIC SOURCE EXTRAPOLATION          -
CD   NZSWP        NUMBER OF AXIAL PARTIAL CURRENT SWEEPS PER       -
CD                GROUP PER OUTER ITERATION (NODAL HEXAGONAL       -
CD                GEOMETRY OPTION)                                -
CD   NCMRZS       NUMBER OF AXIAL COARSE-MESH REBALANCE           -
CD                NUMBER PAIRS (NODAL HEXAGONAL GEOMETRY OPTION) -
CD   IDUM(I)      RESERVED                                        -
C                                                                 -
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR          CONVERGENCE CRITERIA AND OTHER FLOATING POINT DATA     -
CR          (3D RECORD)                                           -
C                                                                 -
CL    EPS1,EPS2,EPS3,EFFK,FISMIN,PSINRM,POWIN,SIGBAR,EFFKQ,       -
CL   1EPSWP,(DUM(I),I=1,20)                                       -
C                                                                 -
CW    30*MULT=NUMBER OF WORDS                                     -
C                                                                 -
CD    EPS1            EIGENVALUE CONVERGENCE CRITERION FOR STEADY -
CD                    STATE CALCULATION                           -
CD    EPS2            POINTWISE FISSION SOURCE CONVERGENCE CRITERION -
CD                    FOR STEADY STATE SHAPE CALCULATION          -
CD    EPS3            AVERAGE FISSION SOURCE CONVERGENCE CRITERION -
CD                    FOR STEADY STATE SHAPE CALCULATION          -
CD    EFFK            K-EFFECTIVE OF REACTOR                      -
CD    FISMIN          ANY POINTWISE FISSION SOURCE WILL BE NEGLECTED -
CD                    IN THE POINTWISE FISSION SOURCE CONVERGENCE  -
CD                    TEST IF IT IS LESS THAN THIS FACTOR TIMES    -
CD                    THE R.M.S. FISSION SOURCE                   -
CD    PSINRM          ERROR REDUCTION FACTOR TO BE ACHIEVED BY EACH -
CD                    SERIES OF INNER ITERATIONS FOR EACH GROUP    -
CD                    DURING A SHAPE CALCULATION                  -
CD    POWIN           STEADY STATE REACTOR POWER (WATTS)          -
CD    SIGBAR          DOMINANCE RATIO                             -
CD    EFFKQ           EIGENVALUE OF THE HOMOGENEOUS PROBLEM       -
CD                    CORRESPONDING TO THE NEAR CRITICAL          -
CD                    SOURCE PROBLEM. (PERTINENT WHEN NOUTBQ.GT.0) -
CD    EPSWP           LINE SWEEP CONVERGENCE CRITERION (TRANSPORT  -
CD                    OPTION)                                     -
CD    DUM(I)          RESERVED                                    -
C                                                                 -
C-----------------------------------------------------------------

C-----------------------------------------------------------------
CR          OPTIMUM OVERRELAXATION FACTORS (4D RECORD)            -
C                                                                 -
CC          PRESENT IF NUMORP.GT.0                                -
C                                                                 -
CL    (OMEGA(I),I=1,NUMORP)                                       -
C                                                                 -
CW    NUMORP*MULT=NUMBER OF WORDS                                 -
C                                                                 -
CD    OMEGA(I)          OPTIMUM OVERRELAXATION FACTOR FOR GROUP I -
CD                      ON THIS FILE, OPTIMUM OVERRELAXATION FACTORS -
CD                      ARE --ALWAYS-- ORDERED BY THE --REAL PROBLEM-- -
```

```
CD                    ORDERING                                              -
C                                                                           -
C-------------------------------------------------------------------------
```

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C-------------------------------------------------------------------------
CR          AXIAL COARSE-MESH REBALANCE BOUNDARIES FOR NODAL                -
CR          HEXAGONAL GEOMETRY OPTION (5D RECORD)                           -
C                                                                           -
CC          PRESENT IF NCMRZS.GT.0                                          -
C                                                                           -
CL    (ZCMRC(I),I=1,NCMRZS),(NZINTS(I),I=1,NCMRZS)                          -
C                                                                           -
CW    NCMRZS*(MULT+1)=NUMBER OF WORDS                                       -
C                                                                           -
CD    ZCMRC(I)          UPPER Z-COORDINATE OF AXIAL COARSE-MESH             -
CD                      REBALANCE SPECIFICATION INTERVAL I.                 -
CD    NZINTS(I)         NUMBER OF AXIAL COARSE MESH REBALANCE INTERVALS-
CD                      IN I-TH SPECIFICATION INTERVAL.                     -
C                                                                           -
CN              THERE ARE NZINTS(I) AXIAL COARSE-MESH REBALANCE             -
CN              INTERVALS BETWEEN ZCMRC(I-1) AND ZCMRC(I), WHERE            -
CN              WHERE ZCMRC(0) IS THE LOWER REACTOR BOUNDARY                -
CN              IN THE Z-DIRECTION. THE ZCMRC(I) ARE ORDERED SUCH           -
CN              THAT ZCMRC(I+1).GT.ZCMRC(I).                                -
C                                                                           -
C-------------------------------------------------------------------------
```

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CEOF
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D.3 LABELS

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C***************************************************************************
C                       PREPARED 2/21/78 AT ANL                             -
C                       LAST REVISED 12/12/83                               -
C                                                                           -
CF          LABELS                                                          -
C                                                                           -
CF          REGION AND COMPOSITION LABELS, AREA DATA,                       -
CF          HALF HEIGHTS, NUCLIDE SET LABELS, ALIAS ZONE LABELS,            -
CF          CONROL-ROD MODEL DATA                                           -
C                                                                           -
C***************************************************************************
```

```
C-------------------------------------------------------------------------
CR          FILE IDENTIFICATION                                             -
C                                                                           -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                           -
C                                                                           -
CW    1+3*MULT=NUMBER OF WORDS                                              -
C
```

```
CD    HNAME             HOLLERITH FILE NAME - LABELS - (A6)                 -
CD    HUSE(I)           HOLLERITH USER IDENTIFICATION (A6)                  -
CD    IVERS             FILE VERSION NUMBER                                 -
CD    MULT              DOUBLE PRECISION PARAMETER                          -
CD                          1 - A6 WORD IS SINGLE WORD                      -
CD                          2 - A6 WORD IS DOUBLE PRECISION WORD            -
C                                                                           -
C-------------------------------------------------------------------------
```

```
C-------------------------------------------------------------------------
CS          FILE STRUCTURE                                                  -
CS                                                                          -
CS          RECORD TYPE                       PRESENT IF                    -
CS          ================================  ==============              -
CS          FILE IDENTIFICATION               ALWAYS                        -
CS          SPECIFICATIONS                    ALWAYS                        -
CS          LABEL AND AREA DATA               ALWAYS                        -
CS          FINITE-GEOMETRY TRANSVERSE        NHTS1.GT.0 OR                 -
CS            DISTANCES                        NGTS2.GT.0                   -
CS          NUCLIDE SET LABELS                NSETS.GT.1                    -
CS          ALIAS ZONE LABELS                 NALIAS.GT.0                   -
CS          GENERAL CONTROL-ROD MODEL DATA    NBANKS.GT.0                   -
CS                                                                          -
CS    ************(REPEAT FOR ALL BANKS)                                    -
CS    *     CONTROL-ROD BANK DATA             NBANKS.GT.0                   -
CS    *                                                                     -
CS    *  *******(REPEAT FOR ALL RODS IN BANK)                               -
CS    *  *  CONTROL-ROD CHANNEL DATA          (LLCHN+LLROD+MMESH).GT.0-
CS    **********                                                            -
C                                                                           -
C-------------------------------------------------------------------------
```

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C-------------------------------------------------------------------------
CR          SPECIFICATIONS (1D RECORD)                                      -
C                                                                           -
CL    NTZSZ,NREG,NAREA,LREGA,NHTS1,NHTS2,NSETS,NALIAS,NTRI,NRING,           -
CL    NCHAN,NBANKS,LINTAX,MAXTIM,MAXROD,MAXMSH,MAXLRD,MAXLCH,               -
CL    (IDUM(I),I=1,6)                                                       -
C                                                                           -
CW    24=NUMBER OF WORDS                                                    -
C                                                                           -
CD    NTZSZ             NUMBER OF ZONES AND SUBZONES                        -
CD    NREG              NUMBER OF REGIONS                                   -
CD    NAREA             NUMBER OF AREAS                                     -
CD    LREGA             LENGTH OF NRA ARRAY                                 -
CD    NHTS1             NUMBER OF HALF-HEIGHT AND EXTRAPOLATION             -
CD                      DISTANCE SPECIFICATIONS                             -
CD                         0 - NONE                                         -
CD                         1 - SINGLE VALUE USED EVERYWHERE                 -
CD                         .EQ.NREG - REGION DEPENDENT                      -
CD    NHST2             NUMBER OF HALF-HEIGHT AND EXTRAPOLATION             -
CD                      DISTANCE SPECIFICATIONS FOR THE SECOND              -
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```
CD                    DIRECTION.                                          -
CD                      0 - NONE                                          -
CD                      NHTS1 - SAME AS NHTS1                             -
CD    NSETS           NUMBER OF NUCLIDE SETS                              -
CD    NALIAS          0 IF RECORD 5D IS NOT PRESENT.  IF GREATER          -
CD                    THAN 0, RECORD 5D IS PRESENT AND THE ALIAS          -
CD                    ARRAY IS OF LENGTH NALIAS.                          -
CD    NTRI            NO. OF TRIANGLES PER HEX FOR TRIANGULAR             -
CD                    GOEMETRIES                                          -
CD    NRING           MAX. NO. OF RINGS OF HEXAGONS FOR TRIANGULAR        -
CD                    GEOMETRIES                                          -
CD    NCHAN           NO. OF CONTROL-ROD CHANNELS IN THE MODEL            -
CD    NBANKS          NO. OF CONTROL-ROD BANKS                            -
CD    LINTAX          ORIGINAL NO. OF FINE MESH INTERVALS IN AXIAL        -
CD                    DIMENSION                                           -
CD    MAXTIM          MAXIMUM VALUE OF NTIMES(I) (I=1,NBANKS)             -
CD    MAXROD          MAXIMUM VALUE OF NRODS(I) (I=1,NBANKS)              -
CD    MAXMSH          MAXIMUM VALUE OF NMESH(K) (K=1,LRODS;               -
CD                    I=1,NBANKS) WHERE LRODS=NRODS(I)                    -
CD    MAXLRD          MAXIMUM VALUE OF LENROD(K) (K=1,LRODS;              -
CD                    I=1,NBANKS)                                         -
CD    MAXLCH          MAXIMUM VALUE OF LENCHN(K) (K=1,LRODS;              -
CD                    I=1,NBANKS)                                         -
CD    IDUM            RESERVED                                            -
C                                                                         -
CN            THE AXIAL DIMENSION IS Z IN RZ, XYZ, HEX-Z AND              -
CN            TRIANGULAR-Z GEOMETRIES.  IT IS Y IN XY GEOMETRY.           -
CN            NCHAN IS THE SUM OF NRODS (RECORD 6D) OVER ALL CONTROL      -
CN            ROD BANKS.                                                  -
C                                                                         -
C-------------------------------------------------------------------------
```

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C-------------------------------------------------------------------------
CR          LABEL AND AREA DATA (2D RECORD)                               -
C                                                                         -
CL    (CMPNAM(I),I=1,NTZSZ),(REGNAM(I),I=1,NREG),                         -
CL   1(ARANAM(I),I=1,NAREA),                                              -
CL   2(NRA(I),I=1,LREGA),                                                 -
C                                                                         -
CW    MULT*(NTZSZ+NREG+NAREA)+LREGA=NUMBER OF WORDS                       -
C                                                                         -
CD    CMPNAM(I)         ZONE OR SUBZONE LABEL. SUBZONES FOLLOW ZONES      -
CD    REGNAM(I)         REGION LABEL                                      -
CD    ARANAM(I)         AREA LABEL                                        -
CD    NRA(I)            REGION/AREA ASSIGNMENTS. NRA(N(J)) IS THE         -
CD                      NUMBER OF REGIONS IN AREA J. (NRA(I),I=N(J)+1,    -
CD                      N(J+1)-1) IS A LIST OF THE REGION NUMBERS FOR     -
CD                      THOSE REGIONS. N(1)=1. N(J+1)=N(J)+1+NRA(N(J)).   -
CD                      LREGA=SUM (1+NRA(N(J))) FOR J=1,NAREA             -
C                                                                         -
C-------------------------------------------------------------------------
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C-------------------------------------------------------------------------
CR          FINITE-GEOMETRY TRANSVERSE DISTANCES (3D RECORD)              -
C                                                                         -
CC          PRESENT IF NHTS1.GT.0 OR NHTS2.GT.0                           -
C                                                                         -
CL    (HAFHT1(I),I=1,NHTS1),(XTRAP1(I),I=1,NHTS1),                        -
CL   1(HAFHT2(I),I=1,NHTS2),(XTRAP2(I),I=1,NHTS2)                         -
C                                                                         -
CW    2*(NHTS1+NHTS2)=NUMBER OF WORDS                                     -
C                                                                         -
CD    HAFHT1(I)         ACTUAL TRANSVERSE HALF HEIGHT FOR REGION I        -
CD    XTRAP1(I)         TRANSVERSE EXTRAPOLATION DISTANCE FOR             -
CD                      REGION I                                          -
CD    HAFHT2(I)         ACTUAL TRANSVERSE HALF HEIGHT FOR REGION I        -
CD                      IN THE SECOND DIRECTION                           -
CD    XTRAP2(I)         TRANSVERSE EXTRAPOLATION DISTANCE FOR             -
CD                      REGION I IN THE SECOND DIRECTION                  -
C                                                                         -
CN                      IF HAFHTN(I)+XTRAPN(I)=0.0 (N = 1 OR 2)           -
CN                      THE MODEL IS TREATED AS EXTENDING TO              -
CN                      INFINITY IN THE NTH TRANSVERSE DIMENSION.         -
C                                                                         -
C-------------------------------------------------------------------------
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C-------------------------------------------------------------------------
CR          NUCLIDE SET LABELS (4D RECORD)                                -
C                                                                         -
CC          PRESENT IF NSETS.GT.1                                         -
C                                                                         -
CL    (SETISO(I),I=1,NSETS)                                               -
C                                                                         -
CW    MULT*NSETS=NUMBER OF WORDS                                          -
C                                                                         -
CD    SETISO(I)         LABEL OF THE I-TH NUCLIDE SET                     -
C                                                                         -
C-------------------------------------------------------------------------
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```
C-------------------------------------------------------------------------
CR          ALIAS ZONE LABELS (5D RECORD)                                 -
C                                                                         -
CC          PRESENT IF NALIAS .GT. 0                                      -
C                                                                         -
CL    (ALIAS(I),I=1,NALIAS)                                               -
C                                                                         -
CW    MULT*NALIAS=NUMBER OF WORDS                                         -
C                                                                         -
CD    ALIAS(I)          ALIAS ZONE LABELS                                 -
C                                                                         -
CN                      WHEN RUNNING REBUS-3, THE ZONES ARE               -
CN                      PROLIFERATED TO THE REGIONS AND THE ZONE          -
CN                      LABELS BECOME IDENTICAL TO THE REGION LABELS.     -
CN                      THE ARRAY ALIAS CONTAINS THE LIST OF ORIGINAL     -
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CN                    ZONE LABELS ASSIGNED TO THE VARIOUS REGIONS.   -
C                                                                    -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          GENERAL CONTROL-ROD MODEL DATA (6D RECORD)                -
C                                                                     -
CC          PRESENT IF NBANKS .GT. 0                                  -
C                                                                     -
CL    (BNKLAB(I),I=1,NBANKS),(ZMESHO(I),I=1,LINTAX),                  -
CL    (POSBNK(I),I=1,NBANKS),(NRODS(I),I=1,NBANKS),                   -
CL    (NTIMES(I),I=1,NBANKS),(KFINTO(I),I=1,LINTX1)                   -
C                                                                     -
CW    LINTAX*(MULT+1)+(2*MULT+2)*NBANKS-1=NUMBER OF WORDS             -
C                                                                     -
CD    BNKLAB(I)          CONTROL-ROD BANK LABEL                       -
CD    ZMESHO(I)          ORIGINAL LAST-DIMENSION MESH STRUCTURE       -
CD                       (CM.)                                        -
CD    POSBNK(I)          CURRENT POSITION OF ROD BANK I (CM.)         -
CD    NRODS(I)           NO. OF RODS IN BANK I                        -
CD    NTIMES(I)          NO. OF TIME NODES IN POSITION VS. TIME       -
CD                       TABLE FOR BANK I                             -
CD    KFINTO(I)          ORIGINAL NUMBER OF FINE MESH BETWEEN ZMESHO(I) -
CD                       AND ZMESHO(I+1)                              -
CD    LINTX1             LINTAX-1                                     -
C                                                                     -
CN                       ZMESHO(1)=C.0.  THE ZMESHO ARRAY MUST AT     -
CN                       LEAST CONTAIN ALL THE BOUNDARIES BETWEEN     -
CN                       DISSIMILAR MR ARRAYS (SEE GEODST FILE        -
CN                       DESCRIPTION).  THE ZMESHO ARRAY IN A LABELS   -
CN                       FILE CREATED BY GNIP4C WILL NORMALLY CONTAIN  -
CN                       THE ORIGINAL, COARSE-MESH BOUNDARIES.        -
C                                                                     -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          CONTROL-ROD BANK DATA (7D RECORD)                         -
C                                                                     -
CC          PRESENT IF NBANKS .GT. 0                                  -
C                                                                     -
CL    (RBTIME(J),J=1,LTIME),(RBPOS(J),J=1,LTIME),                     -
CL    (NMESH(K),K=1,LRODS),(LENCHN(K),K=1,LRODS),                     -
CL    (LENROD(K),K=1,LRODS)                                           -
C                                                                     -
CW    2*MULT*LTIME+3*LRODS=NUMBER OF WORDS                            -
C                                                                     -
CD    RBTIME(J)          TIME ENTRIES IN ROD POSITION VS. TIME        -
CD                       TABLE                                        -
CD    RBPOS(J)           ROD-BANK POSITIONS IN TABLE (CM.)            -
CD    NMESH(K)           NO. OF PLANAR MESH CELLS IN ROD K OF CURRENT  -
CD                       ROD BANK                                     -
CD    LENCHN(K)          NO. OF REGIONS DEFINED FOR THE IMMOVEABLE    -
CD                       PORTION OF ROD CHANNEL K                     -
CD    LENROD(K)          NO. OF REGIONS DEFINED FOR THE MOVEABLE      -
CD                       PORTION OF ROD CHANNEL K                     -
CD    LTIME              NTIMES(I) FOR CURRENT ROD BANK               -
CD    LRODS              NRODS(I) FOR CURRENT ROD BANK                -
C                                                                     -
C--------------------------------------------------------------------

C--------------------------------------------------------------------
CR          CONTROL-ROD CHANNEL DATA (8D RECORD)                      -
C                                                                     -
CC          PRESENT IF LLCHN + LLROD + MMESH .GT. 0                   -
C                                                                     -
CL    (POSCHN(L),L=1,LLCHN),(POSROD(L),L=1,LLROD),                    -
CL    (MRCHN(L),L=1,LLCHN),(MRROD(L),L=1,LLROD),                      -
CL    ((MESH(L,M),L=1,ND),M=1,MMESH)                                  -
C                                                                     -
CW    (MULT+1)*(LLROD+LLCHN)+ND*MMESH=NUMBER OF WORDS                 -
C                                                                     -
CD    POSCHN(L)          POSITION (RELATIVE TO THE BOTTOM OF THE MODEL) -
CD                       OF THE LOWER BOUNDARY OF REGION L IN THE     -
CD                       IMMOVEABLE PORTION OF THE CURRENT ROD        -
CD                       CHANNEL (POSCHN(1)=0.0)                      -
CD    POSROD(L)          POSITION (RELATIVE TO ROD TIP) OF THE        -
CD                       LOWER BOUNDARY OF REGION L IN THE MOVEABLE   -
CD                       PORTION OF THE CURENT ROD CHANNEL            -
CD                       (POSROD(1)=0.0)                              -
CD    MRCHN(L)           REGION ASSIGNMENT FOR REGIONS IN THE         -
CD                       IMMOVEABLE PORTION OF THE CURRENT ROD        -
CD                       CHANNEL, STARTING AT THE BOTTOM (Z=0.0)      -
CD                       OF THE MODEL.                                -
CD    MRROD(L)           REGION ASSIGNMENT FOR REGIONS IN THE         -
CD                       MOVEABLE PORTION OF THE ROD, STARTING        -
CD                       WITH THE REGION ADJACENT TO THE ROD TIP      -
CD    LLCHN              LENCHN(K) FOR CURRENT ROD CHANNEL            -
CD    LLROD              LENROD(K) FOR CURRENT ROD CHANNEL            -
CD    MESH(1,M)          1ST DIMENSION INDEX FOR PLANAR MESH CELL M   -
CD                       IN THE CURRENT ROD CHANNEL                   -
CD    MESH(2,M)          2ND DIMENSION INDEX FOR PLANAR MESH CELL M   -
CD                       IN THE CURRENT ROD CHANNEL                   -
CD    ND                 1 IN XY AND RZ GEOMETRIES, 2 IN XYZ, R-THETA-Z,-
CD                       THETA-R-Z, HEX-Z, AND TRIANGULAR-Z MODELS    -
CD    MMESH              NMESH(K) FOR CURRENT ROD CHANNEL             -
C                                                                     -
CN                       NOTE THAT IF NBANKS .GT. 0 BUT LLCHN + LLROD + -
CN                       MMESH .EQ. 0, AN ERROR CONDITION PROBABLY    -
CN                       EXISTS.                                      -
C                                                                     -
C--------------------------------------------------------------------

CEOF
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D.4 NHFLUX

```
C*****************************************************************************
C                       PREPARED  3/01/82                                      -
C                                                                              -
CF          NHFLUX                                                             -
CE          REGULAR NODAL FLUX-MOMENTS AND INTERFACE PARTIAL CURRENTS          -
C                                                                              -
C*****************************************************************************
CD                      ORDER OF GROUPS IS ACCORDING TO DECREASING
CD                      ENERGY. NOTE THAT DOUBLE PRECISION FLUXES ARE
CD                      GIVEN WHEN MULT=2
C------------------------------------------------------------------------------
CS          FILE STRUCTURE                                                     -
CS                                                                             -
CS          RECORD TYPE                    RECORD    PRESENT IF              -
CS          ===========================    ======    ==========              -
CS          FILE IDENTIFICATION                      ALWAYS                  -
CS          SPECIFICATIONS                   1D      ALWAYS                  -
CS                                                                             -
CS  ***********(REPEAT FOR ALL GROUPS)                                        -
CS  *       FLUX MOMENTS                     2D      ALWAYS                  -
CS  *       XY-DIRECTED PARTIAL CURRENTS     3D      ALWAYS                  -
CS  *       Z -DIRECTED PARTIAL CURRENTS     4D      NDIM.EQ.3               -
CS  ***********                                                                -
C                                                                              -
C------------------------------------------------------------------------------
C------------------------------------------------------------------------------
CR          FILE IDENTIFICATION                                                -
C                                                                              -
CL     HNAME,(HUSE(I),I=1,2),IVERS                                             -
C                                                                              -
CW     1+3*MULT=NUMBER OF WORDS                                                -
C                                                                              -
CD     HNAME              HOLLERITH FILE NAME - NHFLUX - (A6)                  -
CD     HUSE(I)            HOLLERITH USER IDENTIFICATION (A6)                   -
CD     IVERS              FILE VERSION NUMBER                                  -
CD     MULT               DOUBLE PRECISION PARAMETER                           -
CD                            1- A6 WORD IS SINGLE WORD                        -
CD                            2- A6 WORD IS DOUBLE PRECISION WORD              -
C                                                                              -
C------------------------------------------------------------------------------
C------------------------------------------------------------------------------
CR          SPECIFICATIONS      (1D RECORD)                                    -
C                                                                              -
CL     NDIM,NGROUP,NINTI,NINTJ,NINTK,ITER,EFFK,POWER,NBLOK,                    -
CL     NMOM,NINTXY,NPCXY                                                       -
C                                                                              -
CW     12 =NUMBER OF WORDS                                                     -
C                                                                              -
CD     NDIM               NUMBER OF DIMENSIONS                                -
CD     NGROUP             NUMBER OF ENERGY GROUPS                             -
CD     NINTI              NUMBER OF FIRST DIMENSION FINE MESH INTERVALS       -
CD     NINTJ              NUMBER OF SECOND DIMENSION FINE MESH INTERVALS      -
CD     NINTK              NUMBER OF THIRD DIMENSION FINE MESH INTERVALS.      -
CD                        NINTK.EQ.1 IF NDIM.LE.2                             -
CD     ITER               OUTER ITERATION NUMBER AT WHICH FLUX WAS            -
CD                        WRITTEN                                             -
CD     EFFK               EFFECTIVE MULTIPLICATION FACTOR                     -
CD     POWER              POWER IN WATTS TO WHICH FLUX IS NORMALIZED           -
CD     NBLOK              DATA BLOCKING FACTOR  (ALWAYS EQUAL TO 1)           -
CD     NMOM               NUMBER OF FLUX MOMENTS IN NODAL APPROXIMATION       -
CD     NINTXY             NUMBER OF MESH CELLS (NODES) ON XY-PLANE            -
CD     NPCXY              NUMBER OF XY-DIRECTED PARTIAL CURRENTS ON           -
CD                        XY-PLANE                                            -
C                                                                              -
C------------------------------------------------------------------------------
C------------------------------------------------------------------------------
CR          REGULAR FLUX MOMENTS   (2D RECORD)                                 -
C                                                                              -
CL     ((FLUX(I,J),I=1,NMOM),J=1,NINTXY)------SEE STRUCTURE BELOW-----         -
C                                                                              -
CW     NMOM*NINTXY*MULT = NUMBER OF WORDS                                      -
C                                                                              -
C      DO 1 K=1,NINTK                                                          -
C    1 READ(N)   *LIST AS ABOVE*                                               -
C                                                                              -
CD     FLUX(I,J)          REGULAR FLUX MOMENTS BY NODE FOR THE PRESENT        -
CD                        GROUP                                               -
C                                                                              -
C------------------------------------------------------------------------------
C------------------------------------------------------------------------------
CR          REGULAR XY-DIRECTED PARTIAL CURRENTS   (3D RECORD)                 -
C                                                                              -
CL     (PCURRH(I),I=1,NPCXY)          ------SEE STRUCTURE BELOW-----           -
C                                                                              -
CW     NPCXY*MULT = NUMBER OF WORDS                                            -
C                                                                              -
C      DO 1 K=1,NINTK                                                          -
C    1 READ(N)   *LIST AS ABOVE*                                               -
C                                                                              -
CD     PCURRH(I)          REGULAR XY-DIRECTED PARTIAL CURRENTS ACROSS ALL-
CD                        XY-PLANE SURFACES FOR THE PRESENT GROUP             -
C                                                                              -
C------------------------------------------------------------------------------
C------------------------------------------------------------------------------
CR          REGULAR  Z-DIRECTED PARTIAL CURRENTS   (4D RECORD)                 -
C                                                                              -
CL     ((PCURRZ(I,J),I=1,NINTXY),J=1,2)-------SEE STRUCTURE BELOW-----         -
C                                                                              -
CW     NINTXY*2*MULT = NUMBER OF WORDS                                         -
C                                                                              -
C      DO 1 K=1,NINTK1                                                         -
C    1 READ(N)   *LIST AS ABOVE*                                               -
C                                                                              -
CC          WITH NINTK1 = NINTK + 1                                            -
C                                                                              -
CD     PCURRZ(I,J)        REGULAR Z-DIRECTED PARTIAL CURRENTS IN              -
```

```
CD                    MINUS- (J=1) AND PLUS- (J=2) Z DIRECTIONS      -
CD                    ACROSS ALL AXIAL BOUNDARIES FOR THE PRESENT    -
CD                    GROUP                                          -
C                                                                    -
C--------------------------------------------------------------------

CEOF
```

D.5 NAFLUX

```
C*********************************************************************
C                     PREPARED  3/01/82                              -
C                                                                    -
CF          NAFLUX                                                   -
CE          ADJOINT NODAL FLUX-MOMENTS AND INTERFACE PARTIAL CURRENTS -
C                                                                    -
C*********************************************************************
CD                    ORDER OF GROUPS IS ACCORDING TO INCREASING
CD                    ENERGY. NOTE THAT DOUBLE PRECISION FLUXES ARE
CD                    GIVEN WHEN MULT=2
C--------------------------------------------------------------------
CS          FILE STRUCTURE                                           -
CS                                                                   -
CS          RECORD TYPE                  RECORD    PRESENT IF        -
CS          ==========================   ======    ==========        -
CS          FILE IDENTIFICATION                    ALWAYS            -
CS          SPECIFICATIONS                 1D      ALWAYS            -
CS                                                                   -
CS  ***********(REPEAT FOR ALL GROUPS)                              -
CS  *       FLUX MOMENTS                   2D      ALWAYS            -
CS  *       XY-DIRECTED PARTIAL CURRENTS   3D      ALWAYS            -
CS  *       Z -DIRECTED PARTIAL CURRENTS   4D      NDIM.EQ.3         -
CS  ***********                                                      -
C                                                                    -
C--------------------------------------------------------------------
C--------------------------------------------------------------------
CR          FILE IDENTIFICATION                                      -
C                                                                    -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                    -
C                                                                    -
CW    1+3*MULT=NUMBER OF WORDS                                       -
C                                                                    -
CD    HNAME             HOLLERITH FILE NAME - NAFLUX - (A6)          -
CD    HUSE(I)           HOLLERITH USER IDENTIFICATION (A6)           -
CD    IVERS             FILE VERSION NUMBER                          -
CD    MULT              DOUBLE PRECISION PARAMETER                   -
CD                          1- A6 WORD IS SINGLE WORD                -
CD                          2- A6 WORD IS DOUBLE PRECISION WORD      -
C                                                                    -
C--------------------------------------------------------------------
C--------------------------------------------------------------------
CR          SPECIFICATIONS     (1D RECORD)                           -
C                                                                    -
CL    NDIM,NGROUP,NINTI,NINTJ,NINTK,ITER,EFFK,ADUM,NBLOK,            -
CL    NMOM,NINTXY,NPCXY                                              -
C                                                                    -
CW    12 =NUMBER OF WORDS                                            -
C                                                                    -
CD    NDIM              NUMBER OF DIMENSIONS                         -
CD    NGROUP            NUMBER OF ENERGY GROUPS                      -
CD    NINTI             NUMBER OF FIRST DIMENSION FINE MESH INTERVALS -
CD    NINTJ             NUMBER OF SECOND DIMENSION FINE MESH INTERVALS -
CD    NINTK             NUMBER OF THIRD DIMENSION FINE MESH INTERVALS. -
CD                      NINTK.EQ.1 IF NDIM.LE.2                      -
CD    ITER              OUTER ITERATION NUMBER AT WHICH FLUX WAS      -
CD                      WRITTEN                                      -
CD    EFFK              EFFECTIVE MULTIPLICATION FACTOR              -
CD    ADUM              RESERVED                                     -
CD    NBLOK             DATA BLOCKING FACTOR  (ALWAYS EQUAL TO 1)    -
CD    NMOM              NUMBER OF FLUX MOMENTS IN NODAL APPROXIMATION -
CD    NINTXY            NUMBER OF MESH CELLS (NODES) ON XY-PLANE     -
CD    NPCXY             NUMBER OF XY-DIRECTED PARTIAL CURRENTS ON    -
CD                      XY-PLANE                                     -
C                                                                    -
C--------------------------------------------------------------------
C--------------------------------------------------------------------
CR          ADJOINT FLUX MOMENTS   (2D RECORD)                       -
C                                                                    -
CL    ((FLUX(I,J),I=1,NMOM),J=1,NINTXY)------SEE STRUCTURE BELOW-----  -
C                                                                    -
CW    NMOM*NINTXY*MULT = NUMBER OF WORDS                             -
C                                                                    -
C     DO 1 K=1,NINTK                                                 -
C   1 READ(N)   *LIST AS ABOVE*                                      -
C                                                                    -
CD    FLUX(I,J)         ADJOINT FLUX MOMENTS BY NODE FOR THE PRESENT -
CD                      GROUP                                        -
C                                                                    -
C--------------------------------------------------------------------
C--------------------------------------------------------------------
CR          ADJOINT XY-DIRECTED PARTIAL CURRENTS   (3D RECORD)       -
C                                                                    -
CL    (PCURRH(I),I=1,NPCXY)          ------SEE STRUCTURE BELOW-----  -
C                                                                    -
CW    NPCXY*MULT = NUMBER OF WORDS                                   -
C                                                                    -
C     DO 1 K=1,NINTK                                                 -
C   1 READ(N)   *LIST AS ABOVE*                                      -
C                                                                    -
CD    PCURRH(I)         ADJOINT XY-DIRECTED PARTIAL CURRENTS ACROSS ALL-
CD                      XY-PLANE SURFACES FOR THE PRESENT GROUP      -
C                                                                    -
C--------------------------------------------------------------------
C--------------------------------------------------------------------
CR          ADJOINT  Z-DIRECTED PARTIAL CURRENTS   (4D RECORD)       -
C                                                                    -
CL    ((PCURRZ(I,J),I=1,NINTXY),J=1,2)------SEE STRUCTURE BELOW-----  -
C                                                                    -
```

Appendix E

LINK EDIT INSTRUCTIONS FOR IBM 370 SYSTEMS

```
//LINKIBM JOB USER=B20245,
//     CLASS=W,TIME=5,REGION=1000K,MSGCLASS=W
//*
//* ***************************************************************
//*
//*   THIS JOB LINK EDITS THE LOAD MODULES STP021 AND SIOSUB IN
//*   THE LIBRARY &NESCLIB.
//*   THE JOB RUNS IN A REGION SIZE OF 1000K.
//*
//* ***************************************************************
//*   EXECUTE LINKAGE EDITOR.
//* ***************************************************************
//STEP1   EXEC PGM=IEWL,PARM='DCBS,LIST,MAP,OVLY,SIZE=(1000K,100K)'
//SYSLIB   DD  DISP=SHR,DSN=SYS1.AMDLIB
//         DD  DISP=SHR,DSN=SYS1.FORTLIB
//SYSLIN   DD  DSN=&OBJECT,DISP=(OLD,DELETE)
//         DD  DDNAME=SYSIN
//SYSLMOD  DD  DSN=&NESCLIB(STP021),
//             DISP=(NEW,CATLG),UNIT=PERM,
//             SPACE=(TRK,(100,20,1),RLSE),DCB=BLKSIZE=6144
//SYSPRINT DD  SYSOUT=A
//SYSUT1   DD  SPACE=(CYL,20),UNIT=(SASCR,SEP=(SYSLIN,SYSLMOD))
//SYSIN DD *
 ENTRY MAIN
 INSERT   LINKR0,LINKR1
 INSERT   REED,SEEK
 INSERT   ERROR,FFORM,FFORM1,FFORM2,LINES,TIMER,SEKPHL
 INSERT   INTSET,FLTSET,IEQUAT,FEQUAT
 INSERT   POINTR,BULK,FREE,IPTERR,WIPOUT,IPT2,PUTM,ILAST,PURGE
 INSERT   ABEND,SQUEZE,INITIO
 INSERT   SIO,RECFM,TRACER,ZEROIO,SIOERR,SIOWU6,SIOTRC
 INSERT   JOBID,SECOND,LOCATE,TABLES,PTERR,LCMSIZ,BFLAGS
 INSERT   PRTI1,PRTI2,PRTR1,PRTR2,PRTECM,STATUS,REDEFM
 INSERT   REDEF,IGET,PUTPNT,GETPNT
 INSERT   TIME,CLOCK#,DATE
 INSERT   JGT,MYLCM,FRELCM,LOCF,LOCFWD,IGTLCM,IGTSCM
 INSERT   IOPUT,PTITLE,ARRAY,STFARC
 OVERLAY LEVEL1
 INSERT   SCAN
 OVERLAY LEVEL1
 INSERT   STUFF,STUFF1
 OVERLAY LEVEL1
 INSERT   GNIP4C,ANIP01,ANIP02,ANIP14,ANIP23,GETZON,GETSZN
 INSERT   BCDFLT,BCDINT,ISIZES
OVERLAY LEVEL2
INSERT   RANIP1
OVERLAY LEVEL3
INSERT   ANIP03,ANIP04,ANIP05,ANIP06
OVERLAY LEVEL3
INSERT   ANIP0X,ANIP07,ANIP09,CHEK09,ANIP10
OVERLAY LEVEL3
INSERT   ANIP11,ANIP12,ANIP15,ANIP34
OVERLAY LEVEL2
INSERT   FGEODS,LOCHEX,SETHEX
OVERLAY LEVEL3
INSERT   GETHGT,GETREG
OVERLAY LEVEL3
INSERT   GETMSH,CMESH,FMESH
OVERLAY LEVEL3
INSERT   GETBUC,GETBC
OVERLAY LEVEL3
INSERT   GETMR,RCMESH,TRIGOM,VOLREG,REDMSH
OVERLAY LEVEL2
INSERT   EGEODS
OVERLAY LEVEL3
INSERT   MAKMSH
OVERLAY LEVEL3
INSERT   PRGEOD,PRNTIX
OVERLAY LEVEL3
INSERT   ANIP43,MPGEOD,MSHMAP
OVERLAY LEVEL3
INSERT   TRIPLT,HEXPIC,HEXPC1,HEXPC2,HEXPC3,HEXPC6,HEXPC7,HEXPC
OVERLAY LEVEL4
INSERT   HEXPC4
OVERLAY LEVEL4
INSERT   HEXPC5
OVERLAY LEVEL3
INSERT   ORTMAP,ORTPC1,ORTPC2,ORTPC3,ORTPC4,ORTPC5,ORTPC6,ORTPC
OVERLAY LEVEL2
INSERT   RANIP2,ANIP13,GETMAT,GETISO,ANIP39,GETSET
OVERLAY LEVEL2
INSERT   FADENS,SORT13,VALU2D,SET2D,INDEX,EDTMAT,SORT14,WNDXSR
OVERLAY LEVEL2
INSERT   BCDXST,RWISOT,RWDELY,RWDY1,RWDY2
OVERLAY LEVEL2
INSERT   WRSRCH
OVERLAY LEVEL3
INSERT   ANIP21,ANIP22,SRCH4D,ANIP24,SRCH3D,ANIP25,SRCH6D,ANIP26
OVERLAY LEVEL3
INSERT   EDSRCH
OVERLAY LEVEL2
INSERT   WRSORC
OVERLAY LEVEL3
INSERT   ANIP19,ANIP40,ANIP41,ANIP42
OVERLAY LEVEL3
INSERT   SORDAT,SORLAB,SORMSH,SORNZN,SORDIF
```

```
OVERLAY LEVEL3
INSERT   ADS,ADS1,ADS2,ADS3
OVERLAY LEVEL3
INSERT   WRS,WRS0,WRS1,WRS2
OVERLAY LEVEL3
INSERT   EDSORC
OVERLAY LEVEL2
INSERT   WRRODS,ANIP44,SORROD,MAKROD,WRTROD,EDTROD
OVERLAY LEVEL1
INSERT   HMG4C
INSERT   REF,HMGPTR
OVERLAY LEVEL2
INSERT   OVL1,RDNDX,EDTISO,IDLR13,ISOR14,RDATDN,ATDN3
OVERLAY LEVEL2
INSERT   OVL2,SCAT,ISOR58,EDTR5,EDTR6,EDTR8,FISPEC,MAXBND,SVSCAT
INSERT   UPDATE,FARSET,ZROSET
OVERLAY LEVEL2
INSERT   OVL3,WREC1,WREC2,WREC3,WREC4
OVERLAY LEVEL2
INSERT   OVL4,SVXS,EDFPWS,EDTXS1,EDTXS2
OVERLAY LEVEL1
INSERT MODCXS,ANIP35,ANIP37,DOMODS,COPIER
OVERLAY LEVEL1
INSERT BCDINP,RADF3D,PDIF3D
OVERLAY LEVEL1
INSERT SRCH4C,GETBSO,GETALP,GETDIM,GETCON,SRCHX,PARAB
INSERT DMDBSQ,DMDALP,DMDDIM,DMDCON,MODBSQ,MODDIM,MODCON
OVERLAY LEVEL1
INSERT   CONTRL,IOCOM,NHIOCM,VERNUM,NHCNTL,SPECS,IOCOMC,IOCOMD
INSERT   NHIOPC,NHIOPD,DEBUG,CFTABL
INSERT   DIF3D,VOLUME,START,WDIF3D,GETBND,AREAS,REVRSE
INSERT   DEFICF,OPENCF,CLOSCF,PURGCF,BLKGET,PNTGET,DEFIDF,OPENDF
INSERT   CLOSDF,STATCF,PCRED
INSERT   LINKR2
OVERLAY LEVEL2
INSERT   BININP,RATFLX,RCMPXS,RDIF3D,RFIXSR,RGEODS,RLABEL,RRTFLX
INSERT   RSEARC,ADSCTM,FORMSH,RNHFLX,RCMPXS,FORMCM
OVERLAY LEVEL2
INSERT   SSINIT,EDITCR
OVERLAY LEVEL3
INSERT   FDINIT,SSCORE,SSDISK
OVERLAY LEVEL3
INSERT ZMINIT,INEDIT,FORMMZ,REGMAP
OVERLAY LEVEL3
INSERT NHINIT,NHGEOM,HEXMAP,GETIJ,NHZMAP,NHPNT,NHCCPT,NHINED,NHCORE
INSERT NHDISK
OVERLAY LEVEL3
INSERT   XSINIT,XSGET1,XSGET2,XSEDIT
OVERLAY LEVEL2
INSERT   SSTATE,SCTSRC,TRISRC,TSWEEP,PSWEEP,TOTSRC,SORINV,ROWSRC
INSERT   FISSRC,OSWEEP,OUTED0,CHEBE,DACOSH,FILCPY,ZEROBA
OVERLAY LEVEL3
INSERT   DXSREV,XSCREV,NHSIGA
OVERLAY LEVEL3
INSERT   DFDCAL,FDCAL,ORTFDC,TRIFDC
OVERLAY LEVEL3
INSERT   FSRCIN,DORPES,ORPES1,ORPES2,RFLXIN,ORPIN1,MLTPLY,ORPIN2
OVERLAY LEVEL3
INSERT   DOUTR1,OUTER1,CHEBY1,INNER1
OVERLAY LEVEL3
INSERT   DOUTR2,OUTER2,CHEBY2,FISSD2,IFISD2,INNER2,SCTSD2,TOTSD2
OVERLAY LEVEL2
INSERT NHSST,NHOEDO,INVERT,NHXSEC
OVERLAY LEVEL3
INSERT DNHCCC,NHCC2D,NHCC3D,NHTVLC,NHINNR
OVERLAY LEVEL3
INSERT DNHSTT,FXREAD,FXINIT,FSINIT
OVERLAY LEVEL3
INSERT DNHOUT,OUTR1,OUTR2,OUTR3,OUTR4,OUTR5,ACCEL,ACCL3D
INSERT LEAK3D,SRCFIS,SRCSCT,SRCHEX,PCHEX,PCHEXB,SRCZ1,SRCZ2,PCZ
INSERT PCZB,FLXHEX,FLXZ,FSUPDT,CMMTRX,BKRING,AXLEAK,CMSOLV,FSERRN
INSERT CONVCK,NHSFCM
OVERLAY LEVEL3
INSERT DNHFIN,NHEDDM,CPYFIL,NHVOL,FXSHAP
OVERLAY LEVEL2
INSERT   DSSTOU,TWODTB,TWODPR,EDITDM,BRED,DSEQUA
INSERT   SCALPK,WPKEDT,NHSHAP,NHPEAK,NHPKED
OVERLAY LEVEL3
INSERT   DSSTO1,BKLWGT,FORMMR,POWINT,SSTOU1,WPOWER,APWADD,RPWADD
INSERT   ORTSRF,TRISRF
OVERLAY LEVEL3
INSERT   DSSTO2,SSTOU2,EDCORE,WFLUX,ORTBAL,RPSADD,TRIBAL
INSERT   WNHFLX,HEXBAL
OVERLAY LEVEL3
INSERT   FLXINT,BALINT,DSSTO3,FLXRZ,ADDVEC,DIVVEC,APSADD,BALBUF
INSERT   ABLADD,RBLADD,RBLFIS,RBLMED,WRZFLX
/*
//* ****************************************************************
//*   EXECUTE LINKAGE EDITOR.
//* ****************************************************************
//STEP7   EXEC PGM=IEWL,PARM='DCBS,LIST,MAP,RENT,SIZE=(230K,100K)'
//SYSLIB   DD  DISP=SHR,DSN=SYS1.AMDLIB
//         DD  DISP=SHR,DSN=SYS1.FORTLIB
//SYSLIN   DD  DSN=&OBJECT,DISP=(OLD,DELETE)
//         DD  DDNAME=SYSIN
//SYSLMOD  DD  DSN=&NESCLIB(SIOSUB),DISP=OLD
//SYSPRINT DD  SYSOUT=A
//SYSUT1   DD  SPACE=(CYL,20),UNIT=(SASCR,SEP=(SYSLIN,SYSLMOD))
```

Appendix F.1

SEGMENTED LOADER INSTRUCTIONS FOR SEGLINK ON THE CDC 7600

```
SEGLD3D,7,400,20000.XXXXXX
:<compile source and pass LGO file to SEGLINK>
.
SFL,170000,100000.
SEGLINK(F=LGO,P=FTN4LIB,B=DIF3D,LO=BEX)
.
.
.
EXIT.

**
**  TREE STRUCTURE DEFINITION WITH IMPLICIT INCLUDES
**
ROOT   TREE   D3DRIV-(SCAN,STUFF,GNIP4,HMG4,MODCXS,BCDINP,SRCH4C,BININP,
,SSINI,SSTAT,NHSS,DSSTO,UDOIT1,UDOIT2,UDOIT3,UDOIT4)
*
GNIP4   TREE GNIP4C-(RNIP1,FGEOD,EGEOD,RANIP2,FADENS,BCDXST,WSRCH,WSORC
,WRRODS)
RNIP1   TREE RANIP1-(ANIP03,ANIPHX,ANIP11)
FGEOD   TREE FGEODS-(GETHGT,GETMSH,GETBUC,GETMR)
EGEOD   TREE EGEODS-(MAKMSH,PRGEOD,ANIP43,HEXMP,ORTMAP)
HEXMP   TREE HEXMAP-(HEXPC4,HEXPC5)
WSRCH   TREE WRSRCH-(ANIP21,EDSRCH)
WSORC   TREE WRSORC-(ANIP19,SORDAT,ADS,WRS,EDSORC)
*
HMG4    TREE HMG4C-(OVL1,OVL2,OVL3,OVL4)
*
SSINI   TREE SSINIT-(FDINIT,ZMINIT,NHINIT,XSINIT)
SSTAT   TREE  SSTATE-(DXSREV,DFDCAL,DORPES,DOUTR1,DOUTR2)
*
NHSS    TREE NHSST-(DNHCCC,DNHSTT,DNHOUT,DNHFIN)
*
DSSTO   TREE  DSSTOU-(DSSTO1,DSSTO2,DSSTO3)
**
**  EXPLICIT SEGMENT DEFINITIONS
**
D3DRIV  INCLUDE  D3DRIV,CRED,DOPC,DRED,DRED1,DRED2,ERROR,FEQUAT,FFORM,EC
,MV,ECZERO,FFORM1,FFORM2,FLTSET,IEQUAT,IGTLCM,JGTSCM,FRELCM,LOCFWD,INTSE
,T,IN2LIT,LINES,POINTR,PUTPNT,BULK,FREE,WIPOUT,GETPNT,IGET,IPT2,PUTM,IPT
,ERR,ILAST,REDEF,REDEFM,PURGE,STATUS,PRTI1,PRTI2,PRTR1,PRTR2,PRTECM,REED
,,ZEROIO,SEEK,SEKPHL,SPACE,SQUEZE,SRLAB,TIMER,DIF3D,START,VOLUME,WDIF3D,
,GETBND,AREAS,REVRSE,DEFICF,OPENCF,CLOSCF,PURGCF,BLKGET,PNTGET,DEFIDF,OP
,ENDF,CLOSDF,STATCF,CODECD,READEC,WRITEC,PCRED
*
STUFF   INCLUDE  STUFF,STUFF1
*
GNIP4C  INCLUDE  GNIP4C,ANIP01,ANIP02,ANIP14,ANIP23,GETZON,GETSZN
ANIP03  INCLUDE  ANIP03,ANIP04,ANIP05,ANIP06
ANIPHX  INCLUDE  ANIPHX,ANIP07,ANIP09,CHEK09,ANIP10
ANIP11  INCLUDE  ANIP11,ANIP12,ANIP15,ANIP34
FGEODS  INCLUDE  FGEODS,LOCHEX,SETHEX
GETHGT  INCLUDE  GETHGT,GETREG
GETMSH  INCLUDE  GETMSH,CMESH,FMESH
GETBUC  INCLUDE  GETBUC,GETBC
GETMR   INCLUDE  GETMR,RCMESH,TRIGOM,VOLREG,REDMSH
PRGEOD  INCLUDE  PRGEOD,PRNTIX
ANIP43  INCLUDE  ANIP43,MPGEOD,MSHMAP
TRIPL   INCLUDE  TRIPLT,HEXPIC,HEXPC1,HEXPC2,HEXPC3,HEXPC6,HEXPC7
ORTMAP  INCLUDE  ORTMAP,ORTPC1,ORTPC2,ORTPC3,ORTPC4,ORTPC5,ORTPC6
RANIP2  INCLUDE  RANIP2,ANIP13,GETMAT,GETISO,ANIP39,GETSET
FADENS  INCLUDE  FADENS,SORT13,VALU2D,SET2D,INDEX,EDTMAT,SORT14,WNDXSR
BCDXST  INCLUDE  BCDXST,RWISOT,RWDELY,RWDY1,RWDY2
ANIP21  INCLUDE  ANIP21,ANIP22,SRCH4D,ANIP24,SRCH3D,ANIP25,SRCH6D,ANIP26
ANIP19  INCLUDE  ANIP19,ANIP40,ANIP41,ANIP42
SORDAT  INCLUDE  SORDAT,SORLAB,SORMSH,SORNZN,SORDIF
ADS     INCLUDE  ADS,ADS1,ADS2,ADS3
WRS     INCLUDE  WRS,WRS0,WRS1,WRS2
WRRODS  INCLUDE  WRRODS,ANIP44,SORROD,SORMSH,SORNZN,SORDIF
*
HMG4C   INCLUDE HMG4C
OVL1    INCLUDE  OVL1,RDNDX,RDATDN,ATDN3,ISOR14,EDTISO,IDLR13
OVL2    INCLUDE  OVL2,ISOR58,SVSCAT,FARSET,ZROSET,UPDATE,MAXBND,FISPEC,E
,DTR5,EDTR6,EDTR8
OVL3    INCLUDE  OVL3,WREC1,WREC2,WREC3,WREC4
OVL4    INCLUDE  OVL4,SVXS,EDTXS1,EDTXS2,EDFPWS
*
MODCXS  INCLUDE  MODCXS,ANIP35,ANIP37,DOMODS,COPIER
*
BCDINP  INCLUDE  BCDINP,RADF3D,PDIF3D
*
SRCH4C  INCLUDE  SRCH4C,GETBSQ,GETALP,GETDIM,GETCON,SRCHX,PARAB,DMDBSQ,D
,MDALP,DMDDIM,DMDCON,MODBSQ,MODDIM,MODCON
*
BININP  INCLUDE  BININP,RDIF3D,RLABEL,RSEARC,RCMPXS,ADSCTM,RGEODS,FORMSH
,,RRTFLX,RATFLX,RFIXSR,RNHFLX,RCMPXS,FORMCM
*
SSINIT  INCLUDE  SSINIT,EDITCR
FDINIT  INCLUDE  FDINIT,SSCORE,SSDISK
ZMINIT  INCLUDE  ZMINIT,INEDIT,FORMMZ,REGMAP
NHINIT  INCLUDE  NHINIT,NHGEOM,HEXMAP,GETIJ,NHZMAP,NHPNT,NHCCPT,NHINED,N
,HCORE,NHDISK
XSINIT  INCLUDE  XSINIT,XSGET1,XSGET2,XSEDIT
*
SSTATE  INCLUDE  SSTATE,CHEBE,DACOSH,OUTEDO,FILCPY,OSWEEP,PSWEEP,TSWEEP
,SORINV,FISSRC,TOTSRC,SCTSRC,ROWSRC,TRISRC,ZEROBA
DXSREV  INCLUDE  DXSREV,XSCREV
DFDCAL  INCLUDE  DFDCAL,FDCAL,ORTFDC,TRIFDC
DORPES  INCLUDE  DORPES,ORPES1,ORPIN1,RFLXIN,FSRCIN,ORPES2,ORPIN2,MLTPLY
DOUTR1  INCLUDE  DOUTR1,OUTER1,INNER1,CHEBY1
DOUTR2  INCLUDE  DOUTR2,OUTER2,INNER2,CHEBY2,IFISD2,SCTSD2,TOTSD2,FISSD2
*
```

```
NHSST   INCLUDE  NHSST,NHOEDO,INVERT,NHXSEC
DNHCCC  INCLUDE  DNHCCC,NHCC2D,NHCC2D,NHCC3D,NHTVLC,NHINNR
DNHSST  INCLUDE  DNHSST,FXREAD,FXINIT,FSINIT
DNHOUT  INCLUDE  DNHOUT,OUTR1,OUTR2,OUTR3,OUTR4,OUTR5,ACCEL,ACCL3D,LEAK3
,D,SRCFIS,SRCSCT,SRCHEX,PCHEX,PCHEXB,SRCZ1,SRCX2,PCZ,PCZB,FLXHEX,FLXZ,FS
,UPDT,CMMTRX,BKRING,AXLEAK,CMSOLV,FSERRN,CONVCK,NHSFCM
DNHFIN  INCLUDE  DNHFIN,NHEDDM,CPYFIL,NHVOL,FXSHAP
*
DSSTOU  INCLUDE  DSSTOU,TWODPR,TWODTR,BRED,DSEQUA,EDITDM,SCALPK,WPKEDT
,NHSHAP,NHPEAK,
DSSTO1  INCLUDE  DSSTO1,FORMMR,BKLWGT,SSTOU1,POWINT,RPWADD,APWADD,WPOWER
,ORTSRF,TRISRF
DSSTO2  INCLUDE  DSSTO2,EDCORE,SSTOU2,RPSADD,WFLUX,ORTBAL,TRIBAL,WNHFLX,
DSSTO3  INCLUDE DSSTO3,ADDVEC,DIVVEC,BALINT,RBLADD,RBLMED,RBLFIS,ABLADD,
,APSADD,FLXINT,FLXRZ,WRZFLX
**
**  GLOBAL COMMON BLOCK DECLARATIONS
**
        GLOBAL  STPARC,PTITLE,IOPUT,ARRAY,VERNUM,IOCOM,SPECS,CONTRL,IOCO
,MD,DEBUG,IOCG4C,SINGLE,POINTS,PNAMES,LOCATE,TNAMES,IDENT,LABSPC,FILEID,
,NHCNTL,NHIOCM,NHIOPC,NHIOPD
GNIP4C  GLOBAL  BCDFLT,BCDINT,ISIZES
HEXMAP  GLOBAL  HEXPC
ORTMAP  GLOBAL  ORTPC
HMG4C   GLOBAL  REF,HMGPTR
DSSTOU  GLOBAL  EDITDM
DSSTO3  GLOBAL  BALBUF
**
**  END OF SEGLINK INPUT
**
      END   03DRIV
```

Appendix F.2

TYPE 01 OVERLAY DIRECTIVES FOR THE LDR LOADER ON THE CRAY-1

```
FILE,$BLD.
OVLDN,DIF3D.
SBCA,????. (ADDRESS OF LONGEST OVERLAY MUST BE OBTAINED FROM LOADER OUTPUT)
ROOT,D3DRIV,CRED,DOPC,DRED,ERROR,FEQUAT,FFORM,FFORM1,FFORM2,FLTSET,
IEQUAT,IGTLCM,JGT,FRELCM,LOCF,LOCFWD,INTSET,IN2LIT,
LINES,POINTR,PUTPNT,BULK,FREE,WIPOUT,GETPNT,IGET,IPT2,PUTM,IPTERR,
ILAST,REDEF,REDEFM,PURGE,STATUS,PRTI1,PRTI2,PRTR1,PRTR2,PRTECM,REED,
ZEROIO,SEEK,SEKPHL,SPACE,SQUEZE,SRLAB,TIMER,DIF3D,START,VOLUME,WDIF3D,
GETBND,AREAS,REVRSE,DEFICF,OPENCF,CLOSCF,PURGCF,BLKGET,PNTGET,DEFIDF,
OPENDF,CLOSDF,STATCF,CODECD,PCRED.
POVL,1,SCAN.
POVL,2,STUFF,STUFF1.
POVL,3,CNIP4C,ANIP01,ANIP02,ANIP14,ANIP23,GETZON,GETSZN,CPYLBG.
SOVL,1,RANIP1,ANIP03,ANIP04,ANIP05,ANIP06,
ANIPHX,ANIP07,ANIP09,CHEK09,ANIP10,
ANIP11,ANIP12,ANIP15,ANIP34.
SOVL,2,FGEODS,LOCHEX,SETHEX,
GETHGT,GETREG,
GETMSH,CMESH,FMESH,SRFLT,
GETBUC,GETBC,
GETMR,RCMESH,TRIGOM,VOLREG,REDMSH.
SOVL,4,EGEODS,MAKMSH,PRGEOD,PRNTIX,
ANIP43,MPGEOD,MSHMAP,
TRIPLT,HEXPIC,HEXPC1,HEXPC2,HEXPC3,HEXPC6,HEXPC7,HEXPC4,HEXPC5,
ORTMAP,ORTPC1,ORTPC2,ORTPC3,ORTPC4,ORTPC5,ORTPC6.
SOVL,4,RANIP2,ANIP13,GETMAT,GETISO,ANIP39,GETSET.
SOVL,5,FADENS,SORT13,VALU2D,SET2D,INDEX,EDTMAT,SORT14,WNDXSR.
SOVL,6,BCDXST,RWISOT,RWDELY,RWDY1,RWDY2.
SOVL,8,WRSRCH,ANIP21,ANIP22,SRCH4D,ANIP24,SRCH3D,ANIP25,SRCH6D,ANIP26,
EDSRCH.
SOVL,7,WRSORC,ANIP19,ANIP40,ANIP41,ANIP42,
SORDAT,SORLAB,SORMSH,SORNZN,SORDIF,
ADS,ADS1,ADS2,ADS3,
WRS,WRS0,WRS1,WRS2,
EDSORC.
POVL,4,HMG4C.
SOVL,1,OVL1,RDNDX,RDATDN,ATDN3,ISOR14,EDTISO,IDLR13.
SOVL,2,OVL2,ISOR58,SVSCAT,FARSET,ZROSET,UPDATE,MAXBND,FISPEC,EDTR5,
EDTR6,EDTR8.
SOVL,3,OVL3,WREC1,WREC2,WREC3,WREC4.
SOVL,4,OVL4,SVXS,EDTXS1,EDTXS2,EDFPWS.
POVL,5,MODCXS,ANIP35,ANIP37,DOMODS,COPIER.
POVL,21,BCDINP,RADF3D,PDIF3D.
POVL,6,SRCH4C,GETBSQ,GETALP,GETDIM,GETCON,SRCHX,PARAB,DMDBSQ,DMDALP,
DMDDIM,DMDCON,MODBSQ,MODDIM,MODCON.
POVL,22,BININP,RDIF3D,RLABEL,RSEARC,RCMPXS,ADSCTM,RGEODS,FORMSH,
FORMCM,RRTFLX,RATFLX,RFIXSR,RNHFLX.
POVL,23,SSINIT,EDITCR.
SOVL,1,FDINIT,SSCORE,SSDISK.
SOVL,2,ZMINIT,INEDIT,FORMMZ,REGMAP.
SOVL,3,NHINIT,NHGEOM,HEXMAP,GETIJ,NHZMAP,NHPNT,NHCCPT,NHINED,NHCORE,
NHDISK.
SOVL,4,XSINIT,XSGET1,XSGET2,XSEDIT.
POVL,24,SSTATE,CHEBE,DACOSH,OUTEDO,FILCPY,OSWEEP,PSWEEP,TSWEEP,
SORINV,FISSRC,TOTSRC,SCTSRC,ROWSRC,TRISRC,ZEROBA,RBOSOR,RBOSRC.
SOVL,1,DXSREV,XSCREV,NHSIGA.
SOVL,2,DFDCAL,FDCAL,ORTFDC,TRIFDC.
SOVL,3,DORPES,ORPES1,ORPIN1,RFLXIN,FSRCIN,ORPES2,ORPIN2,MLTPLY.
SOVL,4,DOUTR1,OUTER1,INNER1,CHEBY1.
SOVL,5,DOUTR2,OUTER2,INNER2,CHEBY2,IFISD2,SCTSD2,TOTSD2,FISSD2.
POVL,25,NHSST,NHOEDO,INVERT,NHXSEC.
SOVL,1,DNHCCC,NHCC2D,NHCC3D,NHTVLC,NHINNR.
SOVL,2,DNHSTT,FXREAD,FXINIT,FSINIT.
SOVL,3,DNHOUT,OUTR1,OUTR2,OUTR3,OUTR4,OUTR5,
ACCEL,ACCL3D,LEAK3D,
SRCFIS,SRCSCT,
SRCHEX,PCHEX,PCHEXB,SRCZ1,SRCZ2,PCZ,PCZB,
FLXHEX,FLXZ,FSUPTD,CMMTRX,BKRING,AXLEAK,
CMSOLV,FSERRN,CONVCK.
SOVL,4,DNHFIN,NHEDDM,CPYFIL,NHVOL,FXSHAP.
POVL,29,DSSTOU,TWODPR,TWODTB,BRED,DSEOUA,SCALPK,WPKEDT,NHSHAP,NHPEAK,
NHPKED.
SOVL,1,DSSTO1,FORMMR,BKLWGT,SSTOU1,POWINT,RPWADD,APWADD,WPOWER,ORTSRF,
TRISRF.
SOVL,2,DSSTO2,EDCORE,SSTOU2,RPSADD,WFLUX,ORTBAL,TRIBAL,WNHFLX,HEXBAL.
SOVL,3,DSSTO3,ADDVEC,DIVVEC,BALINT,RBLADD,RBLMED,RBLFIS,ABLADD,
APSADD,FLXINT,FLXRZ,WRZFLX.
```

Appendix G

SAMPLE PROBLEM OUTPUT

G.1 Sample Problem 1 (entire output)

```
SCAN                                                    1/05/84  2221.700  PAGE   1

BCD INPUT FILE =  5
PRINT FILE =  6
AUXILIARY PRINT FILE = 10


BCD INPUT

BLOCK=STP021
UNFORM=A.DIF3D
01    **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FDD6
02    3600  6000
03    0 0 0 0 30
04    1 0 0 11 111 10 100 1 0 0
06    1.0 0.001 0.04 0.5
UNF.RH=A.NIP3
01    **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FDD6
02    0  1 10000  0  1000  0  0  0  0  1
03    70
04    2 4 0 4
05    XU  .5000  1 4
05    YU  .5000  1 4
07    TOMRE IC OC
07    TTOD   CR CF
07    TOTAL  IC OC BB CR CF
14    M1     I1    1.0
14    M2     I2    1.0
14    M3     I3    1.0
14    M4     I4    1.0
14    M5     I5    1.0
14    M6     I6    1.0
15    M1     IC
15    M2     OC
15    M3     BB
15    M5     CR
15    M6     CF
29    11.2003  11  1
30    IC  1
30    IC  2
30    IC  3
30    IC  4
30    IC  5
30    IC  6
30    OC  6  1
30    OC  7
30    OC  8
30    BB  9
30    BB 10
30    BB  8  1
30    OC  9  4  5
30    OC  9 45 46
30    BB 11  5  6
30    BB 11 56 57
30    CR  7  3
30    CR  7 35
30    CF  4  1
43    1  0  0 .6
MOBOST=A.ISO
 OV ISOTIS  MM2  *CPE 3D BNCH *     1
```

```
SCAN                                                    1/05/84  2221.700  PAGE   2

 1D     4     6     0     3     0     1     1     1
 2D *RA COOLED FBR BENCHMARK FOUR GROUP CROSS SECTIONS                          *
*     *  11    12    13    14    15    16
 0.768      0.232      0.0        0.0
 1.77336E+08 4.02663E+08 7.97003E+07 3.15946E+07 1.05    E+07 8.00    E+05
 10000.      1000.       0.0
     0     3     6     9    12    15
 4D  11      CPE          1
 100.        0.0          0.0          0.0          0.0          0.0
     0     0     1     0     0     0     0     0     1     1     0   200
     1     1     2     3     4     1     1     1     1
 5D .11587      .21220       .46137       .36571       .11587
.21220       .46137       .36571       .69059  E-031.8307582E-01 .92948 E-02
.17305 E-01  .39127 E-02 .18286 E-02 .56336 E-02 .02415 E-02 3.036066
2.912171   2.881874    2.879511
7D 0.0          0.0          .023597      0.0          .16153  E-02
.40791 E-05 0.0          .46838 E-02 .42309 E-07 .44493 E-07
4D  12      CPE          1
100.        0.0          0.0          0.0          0.0          0.0
     0     0     1     0     0     0     0     0     1     1     0   200
     1     1     2     3     4     1     1     1     1
 5D .11586      .21213       .46720       .35369       .11588
.21215       .46720       .35369       .66221 E-031.83956 E-03 1.00354E-02
.70476 E-01  .48531 E-02 .26377 E-02 .51332 E-02 .15238 E-03 3.079043
2.934926   2.8449+5    2.882535
7D 0.0          0.0          .023262      0.0          .15718  E-02
.44451 E-05 0.0          .43614 E-02 .40726 E-07 .49968 E-07
4D  15      CPE          1
100.        0.0          0.0          0.0          0.0          0.0
     0     0     1     0     0     0     0     0     1     1     0   200
     1     1     2     3     4     1     1     1     1
 5D .14584      .28443       .52703       .40732       .14584
.28443       .52703       .40732       1.115278-031.063463E-031.002116E-02
.12999E-01 .27688 E-02 .64367 E-06 .13274 E-03 .34952 E-03 2.796610
2.4402977   2.423171    2.422951
7D 0.0          0.0          .032071      0.0          .17776  E-02
.58880 E-05 0.0          .58971 E-02 .90018 E-07 .45039 E-07
4D  14      CPE          1
100.        0.0          0.0          0.0          0.0          0.0
     0     0     1     0     0     0     0     0     1     1     0   200
     1     1     2     3     4     1     1     1     1
 5D .13270      .23133       .46274       .33749       .13270
.23133       .46274       .33749       8.2278 E-042.17067E-03 7.66083E-03
.97185 E-02 .19453 E-02 .51065 E-04 .07566 E-04 .23769 E-03 2.790264
2.441880   2.423086    2.422988
7D 0.0          0.0          .026322      0.0          .22869  E-02
.28907 E-05 0.0          .53536 E-02 .62133 E-07 .33368 E-07
4D  15      CPE          1
100.        0.0          0.0          0.0          0.0          0.0
     0     0     0     0     0     0     0     0     1     1     0   200
     1     1     2     3     4     1     1     1     1
 5D .13917      .25355       .58044       .5413(8      .13311
.25355       .58044       .54168       .18849E-03 .12643E-01 .63460E-01
.16868
7D 0.0          0.0          .032946      0.0          .37687  E-02
.10320 E-03 0.0          .86815 E-02 .70361 E-11 .10489 E-07
4D  16      CPE          1
100.        0.0          0.0          0.0          0.0          0.0
```

```
SCAN                                                    1/05/84  2221.700  PAGE   3

     0    0    0    0    0    0    0    0    1    1    0  200
     |    |    2    3    4    |    1    |    |
 50 .072206     .11487      .32642      .19272      .072206
 .11487      .32642      .19272      .216305E-03 .16880 E-03 .11468 E-02
 .78660 E-03
 70 0.0          0.0          .012942     0.0          .12871  E-02
 .68780 E-06 0.0          .34533 E-02 .43633 E-11 .69903 E-08
BLOCK=STP021,3
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
REMOVE=DIF3D
MODIFY=A.DIF3D
01    **** SAMPLE PROBLEM 2 ****   2D SNR BENCHMARK - RODS IN - NODAL
02    4000  5700
04    1 0 0 00 111 10 100 1 0 0
11    1 40.0 1 87.5 1 135.0
11    1 175.0
MODIFY=A.NIP3
01    **** SAMPLE PROBLEM 2 ****   2D SNR BENCHMARK - RODS IN - NODAL
02    0  1 10000  0  1000  0  0  0  0  0
03    114
43=DELETE
BLOCK=STP021,3
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
REMOVE=NHFLUX
REMOVE=DIF3D
UNFORM=A.DIF3D
01    **** SAMPLE PROBLEM 3 ****   3D SNR BENCHMARK - RODS IN - NODAL
02    20000  27000 0
03    0 0 0 4500 50
04    1 0 0 00 110 10 100 1 0 0
05    1.0E-7  1.0E-5  1.0E-5
06    1.0 0.001 0.04 0.5
11    1 40.0 1 87.5 1 135.0
11    1 175.0
UNFORM=A.NIP3
01    **** SAMPLE PROBLEM 3 ****   3D SNR BENCHMARK - 8 PLANES - NODAL
02    0  1  8000   0 1000  0  0  0  0  0
03    124
04    7 4 0 4 4 4
05    XU  .5000  1 4
05    YU  .5000  1 4
05    ZL  .5000  1 4
05    ZU  .5000  1 4
09    Z 2 40.0 2 87.5 2 135.0
09    Z 2 175.0
14    M1    I1    1.0
14    M2    I2    1.0
14    M3    I3    1.0
```

```
SCAN                                                    1/05/84  2221.700  PAGE   4

14    M4    I4    1.0
14    M5    I5    1.0
14    M6    I6    1.0
15    M1    IC
15    M2    OC
15    M3    RB
15    M4    AB
15    M5    CR
15    M6    CF
29    11.2003  11  1
30    AB   1  0  0   0.0 175.0
30    IC   1  0  0  40.0 135.0
30    AB   2  0  0   0.0 175.0
30    IC   2  0  0  40.0 135.0
30    AB   3  0  0   0.0 175.0
30    IC   3  0  0  40.0 135.0
30    AB   4  0  0   0.0 175.0
30    IC   4  0  0  40.0 135.0
30    AB   5  0  0   0.0 175.0
30    IC   5  0  0  40.0 135.0
30    AB   6  0  0   0.0 175.0
30    IC   6  0  0  40.0 135.0
30    AB   7  0  0   0.0 175.0
30    OC   7  0  0  40.0 135.0
30    AB   8  0  0   0.0 175.0
30    OC   8  0  0  40.0 135.0
30    RB   9  0  0   0.0 175.0
30    RB  10  0  0   0.0 175.0
30    AB   6  1  1   0.0 175.0
30    OC   6  1  1  40.0 135.0
30    RB   6  1  1   0.0 175.0
30    AB   9  4  5   0.0 175.0
30    OC   9  4  5  40.0 135.0
30    AB   9 45 46   0.0 175.0
30    OC   9 45 46  40.0 135.0
30    RB  11  5  6   0.0 175.0
30    RB  11 56 57   0.0 175.0
30    CF   4  1  1   0.0 135.0
30    CF   7  3  3   0.0  87.5
30    CF   7 35 35   0.0  87.5
30    CR   4  1  1 135.0 175.0
30    CR   7  3  3  87.5 175.0
30    CR   7 35 35  87.5 175.0
BLOCK=STP021,3
REMOVE=GEODST
REMOVE=COMPXS
REMOVE=NDXSRF
REMOVE=ZNATDN
REMOVE=LABELS
REMOVE=RTFLUX
REMOVE=NHFLUX
REMOVE=DIF3D
MODIFY=A.DIF3D
01    **** SAMPLE PROBLEM 4 ****   3D SNR BENCHMARK - RODS IN - FD0636
02    12000 164000
MODIFY=A.NIP3
01    **** SAMPLE PROBLEM 4 ****   3D SNR BENCHMARK - RODS IN - FD0636
03    90
```

```
SCAN                                                    1/05/84  2221.700  PAGE    5

 09     Z 8 40.0 10 87.5 10 135.0
 09     Z 8 175.0
```

```
STUFF                          BCD FILES FORMED FROM BLOCK STP021                    1/05/84  2221.700  PAGE   6

 A.DIF3D   VERSION =  1, MAXIMUM CARD TYPE =   6, NOSORT CARDS =   0
           CARDS-PER-CARD-TYPE =   1   1   1   1   0   1
           THIS FILE CONTAINS UNFORMATTED CARDS.
01     **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FD06
02     3600  6000
03     0 0 0 0 30
04     1 0 0 11 111 10 100 1 0 0
06     1.0 0.001 0.04 0.5


 A.NIP3    VERSION =  1, MAXIMUM CARD TYPE =  43, NOSORT CARDS =   0
           CARDS-PER-CARD-TYPE =  1   1   1   1   2   0   3   0   0   0   0   0   0   6   5   0   0   0   0   0
                                  0   0   0   0   0   0   0   0   1  19   0   0   0   0   0   0   0   0   0   0
                                  0   0   1
           THIS FILE CONTAINS UNFORMATTED CARDS.
01     **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FD06
02     0  1 10000  0  1000  0  0  0  0  1
03     70
04     7 4 0 4
05     XU  .5000  1 4
05     YU  .5000  1 4
07     TCORE IC OC
07     TROD   CR CF
07     TOTAL  IC OC RB CR CF
14     M1     I1    1.0
14     M2     I2    1.0
14     M3     I3    1.0
14     M4     I4    1.0
14     M5     I5    1.0
14     M6     I6    1.0
15     M1     IC
15     M2     OC
15     M3     RB
15     M5     CR
15     M6     CF
29     11.2003  11  1
30     IC  1
30     IC  2
30     IC  3
30     IC  4
30     IC  5
30     IC  6
30     OC  6  1
30     OC  7
30     OC  8
30     RB  9
30     RB 10
30     RB  8  1
30     OC  9  4  5
30     OC  9 45 46
30     RB 11  5  6
30     RB 11 56 57
30     CR  7  3
```

```
STUFF    BCD FILES FORMED FROM BLOCK STP021    1/05/84  2221.700      PAGE   7

 30    CR  7 35
 30    CF  4  1
 43     1  0  0 .6


 A.ISO     VERSION =  1, MAXIMUM CARD TYPE =   0, NOSORT CARDS =  66
           CARDS-PER-CARD-TYPE =   0
 0V ISOTXS  HH2  *GFK 3D BNCH *     1
 1D      4     6     0     3     0     1     1     1
 2D *NA COOLED FBR BENCHMARK FOUR GROUP CROSS SECTIONS                  *
*      * I1     I2     I3     I4     I5     I6
 0.768      0.232      0.0          0.0
 1.72336E+09 4.02463E+08 7.97003E+07 3.15946E+07 1.05   E+07 8.00   E+05
 10000.       1000.        0.0
    0     3     6     9    12    15
 4D  I1     GFK          1
 100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
 5D .11587       .21220       .46137       .34571       .11587
.21220       .46137       .34571       .69059  E-031.830758E-03 .92948 E-02
.17305 E-01 .39123 E-02 .18286 E-02 .36334 E-02 .92415 E-02 3.036066
2.912173    2.881874    2.879511
7D 0.0          0.0          .023597      0.0          .16153  E-02
.40791 E-05 0.0          .46838 E-02 .42309 E-07 .44493 E-07
4D  I2     GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .11588       .21213       .46770       .35349       .11588
.21213       .46770       .35349       .66221 E-031.83956 E-03 1.00354E-02
.20476 E-01 .48531 E-02 .26377 E-02 .51332 E-02 .13238 E-01 3.079063
2.914926    2.884945    2.882535
7D 0.0          0.0          .023262      0.0          .15718  E-02
.46451 E-05 0.0          .43414 E-02 .40724 E-07 .49968 E-07
4D  I3     GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .14584       .28443       .52703       .40732       .14584
.28443       .52703       .40732       1.11527E-033.063463E-031.002116E-02
.129995E-01 .27688 E-02 .44347 E-04 .12274 E-03 .34952 E-03 2.796410
2.440977    2.423171    2.422951
7D 0.0          0.0          .032071      0.0          .27776  E-02
.38880 E-05 0.0          .58971 E-02 .90018 E-07 .45039 E-07
4D  I4     GFK          1
100.        0.0          0.0          0.0          0.0          0.0
    0     0     1     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
5D .12270       .23133       .46274       .33749       .12270
.23133       .46274       .33749       8.2278 E-042.170873E-03 7.64083E-03
.97185 E-02 .19453 E-02 .31065 E-04 .87566 E-04 .23769 E-03 2.790264
2.441880    2.423086    2.422988
7D 0.0          0.0          .026322      0.0          .21889  E-02
.28907 E-05 0.0          .53536 E-02 .62133 E-07 .33248 E-07
4D  I5     GFK          1


STUFF      BCD FILES FORMED FROM BLOCK STP021      1/05/84  2221.700  PAGE   8

 100.        0.0          0.0          0.0          0.0          0.0
    0     0     0     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
 5D .13317       .25355       .58044       .54168       .13317
 .25355       .58044       .54168       .186696E-02 .126433E-01 .634405E-01
 .16868
 7D 0.0          0.0          .022946      0.0          .37687  E-02
 .10320 E-05 0.0          .86815 E-02 .70361 E-11 .10489 E-07
 4D  I6     GFK          1
 100.        0.0          0.0          0.0          0.0          0.0
    0     0     0     0     0     0     0     0     1     1     0   200
    1     1     2     3     4     1     1     1     1
 5D .072206      .11487       .32642       .19272       .072206
 .11487       .32642       .19272       .216305E-03 .16880 E-03 .11468 E-02
 .78660 E-03
 7D 0.0          0.0          .012942      0.0          .12871  E-02
 .68780 E-06 0.0          .34533 E-02 .43633 E-11 .69903 E-08

 SUBROUTINE STUFF USED  2048 WORDS OF CORE
 CP TIME=  0.38 SECONDS, PP TIME=  0.0  SECONDS
```

*** GNIP4C - GENERAL NEUTRONICS BCD INPUT PROCESSOR TO CREATE CCCC BINARY INTERFACE FILES ***

*** GNIP4C CONTROL PARAMETERS ***

10000	IMAING	NO. OF WORDS OF MAIN MEMORY REQUESTED
0	IBULKG	NO. OF WORDS OF BULK MEMORY REQUESTED
0	IPRNTG	BPOINTER TRACE AND DUMP CONTROL (0/1/2/3, NEITHER/DUMP/TRACE/BOTH)
1	IGMEDT	GEOMETRY PROCESSING EDIT CONTROL (0/1/2/3, NO EDITS/PRINT EDITS/EDITS TO AUXILIARY FILE/BOTH)
0	IMAPR	REGION MAP OPTION (0/1/2/3, NO MAP/PRINT MAP/MAP TO AUXILIARY FILE/BOTH)
1	IMAPZ	ZONE (COMPOSITION) MAP OPTION (0/1/2/3, SEE IMAPR)

*** MODEL DESCRIPTION ***

9	IGOM	GEOMETRY TYPE, TRIANGULAR
6	NZONE	NO. OF ZONES (COMPOSITIONS)
5	NREG	NO. OF REGIONS
1	NZCL	NO. OF ZONE CLASSIFICATIONS
31	NCINTI	NO. OF 1ST DIMENSION COARSE MESH INTERVALS
16	NCINTJ	NO. OF 2ND DIMENSION COARSE MESH INTERVALS
31	NINTI	NO. OF 1ST DIMENSION FINE MESH INTERVALS
16	NINTJ	NO. OF 2ND DIMENSION FINE MESH INTERVALS
4	IMB1	FIRST BOUNDARY CONDITION, FIRST DIMENSION, PERIODIC, NEXT FACE CLOCKWISE
2	IMB2	LAST BOUNDARY CONDITION, FIRST DIMENSION, EXTRAPOLATED
	JMB1	FIRST BOUNDARY CONDITION, SECOND DIMENSION, PERIODIC, SEE IMB1
2	JMB2	LAST BOUNDARY CONDITION, SECOND DIMENSION, EXTRAPOLATED
1	NBS	NO. OF BUCKLING SPECIFICATIONS
24	NBCS	NO. OF CONSTANTS FOR EXTERNAL BOUNDARIES
1	NIBCS	NO. OF CONSTANTS FOR INTERNAL BOUNDARIES
0	NZWBB	NO. OF BLACKNESS THEORY ZONES
0	NRASS	0/1, REGION ASSIGNMENTS TO COARSE/FINE MESH
1	NTRIAG	OUTER BOUNDARY SHAPE, 60 DEGREE RHOMBUS
1	NTHPT	ORIENTATION OF (1,1) MESH TRIANGLE - POINTS AWAY FROM 1ST DIMENSION AXIS
1.1200D+01	FLAT	HEXAGON FLAT-TO-FLAT DISTANCE
6.4665D+00	SIDE	LENGTH OF MESH-TRIANGLE SIDE

EXTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
LAST VALUE SHOWN IS USED FOR REMAINING GROUPS

LAST TRIAG BOUNDARY

1 5.00000D-01 2 5.00000D-01 3 5.00000D-01 4 5.00000D-01

LAST BOUNDARY

1 5.00000D-01 2 5.00000D-01 3 5.00000D-01 4 5.00000D-01

REGION/ZONE SPECIFICATIONS

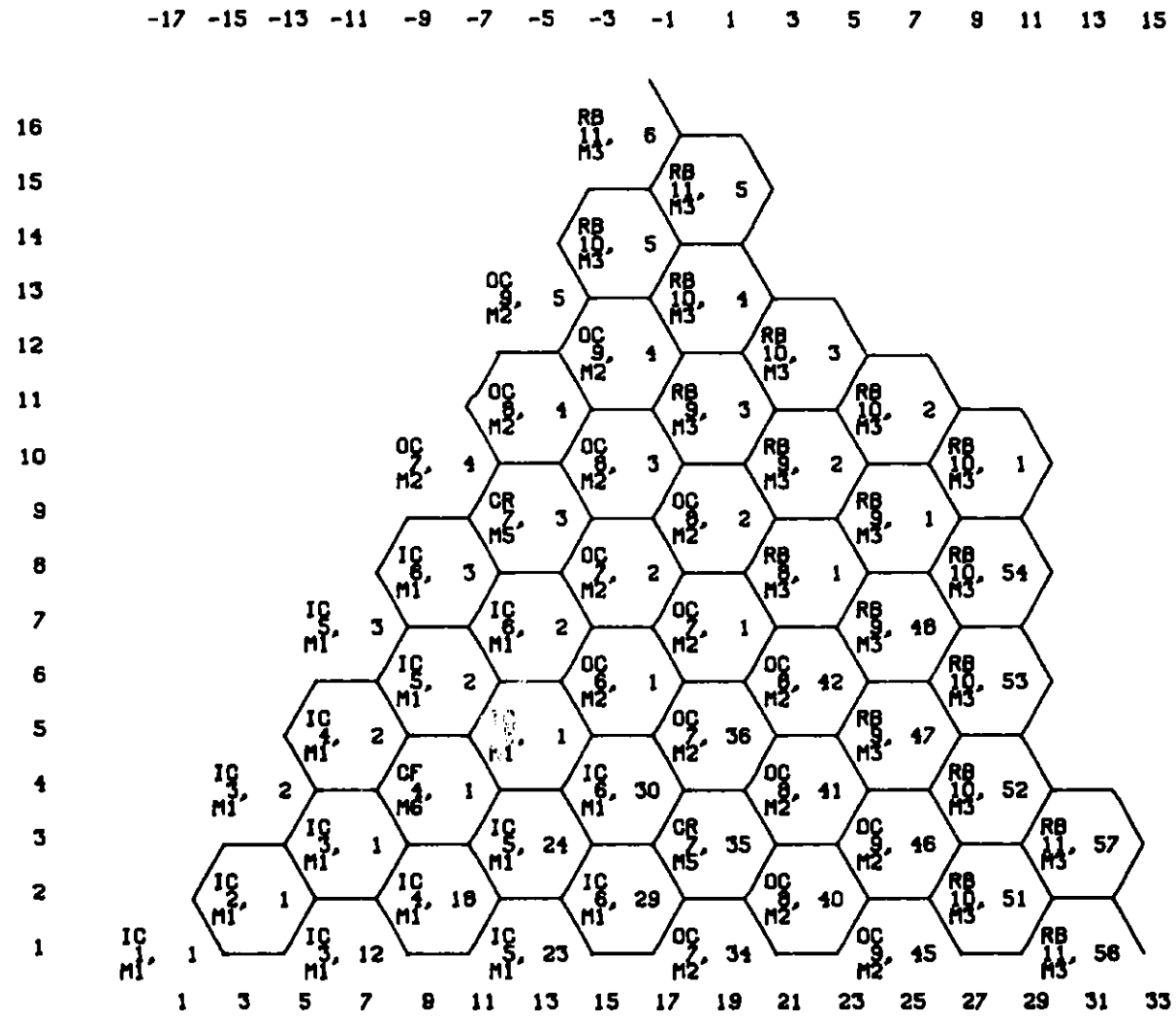
REGION NO.	REGION NAME	REGION VOLUME	ZONE NO.	ZONE NAME	ZONE CLASS.	BUCKLING BY GROUP (REPEAT LAST VALUE FOR REMAINING GROUPS)
1	IC	1.430E+03	1	M1	0	0.0
2	OC	1.521E+03	2	M2	0	0.0
3	RB	1.955E+03	3	M3	0	0.0
4	CR	2.173E+02	5	M5	0	0.0
5	CF	1.086E+02	6	M6	0	0.0

INTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
LAST VALUE SHOWN IS USED FOR REMAINING GROUPS

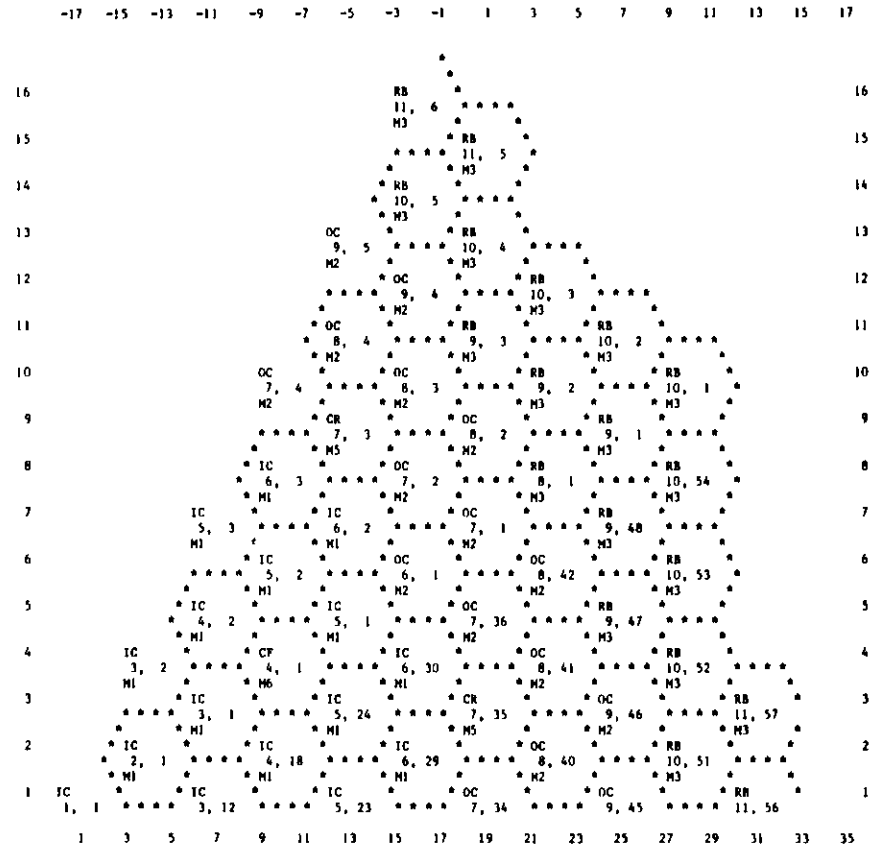
1 0.0

REGIONS COMPRISING AREAS

AREA NO.	NAME	REGION NO.	NAME	REGION NO.	NAME	REGION NO.	NAME	REGION NO.	NAME	REGION NO.	NAME	REGION NO.	NAME
1	TCORE	1	IC	2	OC								
2	TROD	4	CR	5	CF								
3	TOTAL	1	IC	2	OC	3	RB	4	CR	5	CF		



GN1P4C Generated Calcomp 780 Plot of 2D SNR Benchmark Model



*** GRAPHICS OUTPUT SPECIFICATIONS ***

1	IPLOT	0/1, NO GRAPHICS OUTPUT/GRAPHICS OUTPUT
7.8488D+00	XPAGE	WIDTH OF GRAPHICS PAGE (INCHES)
6.2000D+00	YPAGE	HEIGHT OF GRAPHICS PAGE (INCHES)
6.0000D-01	FTOF	FLAT-TO-FLAT DISTANCE (INCHES)
		GRAPHICS COMPLETE

*** ISOTXS FILE CONTROL INFORMATION ***

	HSETID	NA COOLED FBR BENCHMARK FOUR GROUP CROSS SECTIONS
4	NGROUP	NUMBER OF ENERGY GROUPS IN SET
6	NISO	NUMBER OF ISOTOPES IN SET
0	MAXUP	MAXIMUM NUMBER OF UPSCATTER GROUPS
3	MAXDN	MAXIMUM NUMBER OF DOWN SCATTER GROUPS
0	MAXORD	MAXIMUM SCATTERING ORDER
1	ICHIST	FISSION SPECTRUM FLAG
1	NSCMAX	MAXIMUM NO. OF BLOCKS OF SCATTERING DATA
1	NSBLOK	BLOCKING CONTROL FOR SCATTER MATRICES

*** ISOTXS ISOTOPE LABELS ***

ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL	ISOTOPE NO.	LABEL
1	I1	2	I2	3	I3	4	I4	5	I5	6	I6				

*** NDXSRP CONTROL PARAMETERS ***

6	NON	NUMBER OF NUCLIDES
1	NSN	NUMBER OF NUCLIDE SETS
6	NNS	MAXIMUM NUMBER OF NUCLIDES IN A SET
6	NAN	NUMBER OF UNIQUE ISOTOPES
0	NUMMAT	NUMBER OF MATERIALS SPECIFIED
0	NSZ	NUMBER OF SUBZONES SPECIFIED
6	NZONE	NUMBER OF ZONES SPECIFIED

*** DESCRIPTION OF NUCLIDE SET 1 ***

ISOTOPES INCLUDED	I1	I2	I3	I4	I5	I6
ZONES ASSIGNED	M1	M2	M3	M4	M5	M6

CONTENTS OF ZNATDN SPECIFICATIONS RECORD

0.0	TIME	REFERENCE REAL TIME, DAYS
0	NCY	REFERENCE CYCLE NUMBER
6	NTZSZ	NUMBER OF ZONES PLUS NUMBER OF SUBZONES
6	NNS	MAXIMUM NUMBER OF NUCLIDES IN ANY SET
1	NBLKAD	NUMBER OF BLOCKS OF ATOM DENSITY DATA

*** ATOM DENSITIES OF ZONES (INCLUDING CONTRIBUTIONS FROM SUBZONES) ***
THE ISOTOPE NUMBERS SHOWN ARE THE ISOTXS NUCLIDE NUMBERS

ZONE NO.	NAME	NUCLIDE SET	ISOTOPE NO.	NAME	ATOM DENSITY (ATOMS/B-CM)	ISOTOPE NO.	NAME	ATOM DENSITY (ATOMS/B-CM)	ISOTOPE NO.	NAME	ATOM DENSITY (ATOMS/B-CM)	ISOTOPE NO.	NAME	ATOM DENSITY (ATOMS/B-CM)
1	M1		1	I1	1.0000D+00									
2	M2		2	I2	1.0000D+00									
3	M3		3	I3	1.0000D+00									
4	M4		4	I4	1.0000D+00									
5	M5		5	I5	1.0000D+00									
6	M6		6	I6	1.0000D+00									

*** THE FOLLOWING BINARY FILES HAVE BEEN WRITTEN ***

FILE NAME	VERSION NO.	LOGICAL UNIT
ISOTXS	1	27
GEODST	1	26
LABELS	1	20
ZNATDN	1	29
NDXSRF	1	28

ELAPSED CP TIME = 0.86 SECONDS
ELAPSED PP TIME = 0.0 SECONDS
MAIN CORE REQUIRED = 542 WORDS
MAIN CORE REQUESTED = 10000 WORDS
BULK CORE REQUIRED = 0 WORDS
BULK CORE REQUESTED = 0 WORDS

```
HMG4C   6/83     **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FD06     1/05/84  2221.900  PAGE  15
                        * * * HMG4C - CCCC TO ARC SYSTEM CROSS SECTION HOMOGENIZATION * * *

 TIME,     2221.900
 DATE,      1/05/84

 FILE A.HMG4C  DOES NOT EXIST . . . DEFAULT VALUES WILL BE USED
 FILE NDXSRF IS LUN  28 AND CONTAINS THE USER ID - 1/05/2221.9-
 FILE ZNATDN IS LUN  29 AND CONTAINS THE USER ID - 1/05/2221.7-
 FILE ISOTXS IS LUN  27 AND CONTAINS THE USER ID -GFK 3D BNCH -
 FILE COMPXS   WILL NOW BE WRITTEN ON LUN  19

 SIZE OF CONTAINER ALLOCATED FOR HMG4C -   1000
 SIZE OF CONTAINER ACTUALLY USED BY HMG4C -   415

 ELAPSED CPU TIME =     2.14 SEC.
 ELAPSED PP  TIME =     0.0  SEC.
                                                * * * END OF HMG4C * * *


DIF3D 4.0   7/83     **** SAMPLE PROBLEM 1 ****   2D SNR BENCHMARK - RODS IN - FD06     1/05/84  2222.000  PAGE  16
                    INPUT FILE DIF3D , VERSION   1, USER IDENTIFICATION =            HAS BEEN PROCESSED.
                    INPUT FILE COMPXS, VERSION   1, USER IDENTIFICATION =            HAS BEEN PROCESSED.
                    INPUT FILE GEODST, VERSION   1, USER IDENTIFICATION =  1/05/     HAS BEEN PROCESSED.
                    INPUT FILE LABELS, VERSION   1, USER IDENTIFICATION =  1/05/     HAS BEEN PROCESSED.
```

PROCEDURE PARAMETERS	DEFAULT CYLINDERS	RECOMMENDED CYLINDERS	DISK TYPE
ZONCYL	1	1	3330
FLXCYL	1	1	3330
PSICYL	5	1	3330
FDCCYL	20	1	3330
PSUCYL	3	0	3330
SRFCYL	12	1	3330
DMY1CYL	21	2	3330
DMY2CYL	7	3	3330
DMY5CYL	4	1	3330
RTCYL	5	1	3350
ATCYL	5	1	3350

*** DIF3D STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	3600	6000
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH ALL DATA FOR 1 GROUP IN CORE	=	417	4289
WITH SCATTERING BAND OF FLUXES IN CORE	=	417	5777
WITH ALL FILES IN CORE	=	417	10953

LOCATION OF SCRATCH FILES DURING STEADY STATE CALCULATION

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NEW FISSION SOURCE	1	496	496	CORE	1
OLD FISSION SRC. 1	1	496	496	CORE	1
OLD FISSION SRC. 2	1	496	496	DISK	0
TOTAL SOURCE	1	496	496	CORE	1
COMPOSITION MAP	1	248	248	CORE	1
FLUX ITERATE	4	496	1984	CORE	4
CROSS SECTIONS	4	72	288	CORE	4
FINITEDIFF. COEFS.	4	1488	5952	DISK	1

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM	=	417	5993

*** USER INPUT SPECIFICATIONS FOR THIS PROBLEM ***

0	IPROBT	0/1	EIGENVALUE/FIXED SOURCE PROBLEM
0	ISOLNT	0/1	REAL/ADJOINT SOLUTION
0	IXTRAP	0/1	YES/NO CHEBYSHEV OUTER ACCELERATION
0	IRSTRT	0/1	NO/YES THIS IS A RESTART
0	IOSAVE	0/1	NO/YES BYPASS LAST CONCURRENT INNER ITERATION PASS IN GROUPS BELOW THE LAST PASS THRESHOLD
0	IOMEG	0/1	NO/YES ASYMPTOTIC EXTRAPOLATION DURING THE OPTIMUM OVERRELAXATION FACTOR ESTIMATION ITERATIONS

STORAGE, ITERATION, TIME LIMITS

3600	MAXSIZ	NO. OF WORDS REQUESTED FOR FCM DATA STORAGE CONTAINER
6000	MAXBLK	NO. OF WORDS REQUESTED FOR ECM DATA STORAGE CONTAINER
4500	MINBSZ	MINIMUM DESIRED (PLANE-BLOCK) RECORD LENGTH (IN WORDS) FOR CONCURRENT INNER ITERATION
30	NOUTMX	MAXIMUM NUMBER OF OUTER ITERATIONS ALLOWED(-1/-2 BYPASS OUTERS/AND SLOR FACTOR CALCULATION)
1000000000	LIMTIM	MAXIMUM PROCESSOR TIME (SECONDS) ALLOWED
50	INRMAX	MAXIMUM NUMBER OF ITERATIONS PERMITTED DURING THE OPTIMUM OVERRELAXATION FACTOR ESTIMATION PROCEDURE.

EDIT OPTIONS (REGION INTEGRAL EDITS INCLUDE AREA EDITS)

1	IEDF(1)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH PROBLEM DESCRIPTION
0	IEDF(2)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH GEOMETRY REGION MAP
0	IEDF(3)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH GEOMETRY ZONE MAP
11	IEDF(4)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH MACROSCOPIC CROSS SECTIONS (SCATTERING+PRINCIPAL, PRINCIPAL ONLY)
111	IEDF(5)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH BALANCE INTEGRALS BY (GROUP, REGION AND GROUP, REGION)
10	IEDF(6)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH POWER (REGION INTEGRALS, DENSITY BY MESH CELL)
100	IEDF(7)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH FLUX (REGION INTEGRALS, BY MESH CELL, BY MESH CELL AND GROUP)
1	IEDF(8)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH ZONE AVERAGED FLUX
0	IEDF(9)	0/1/2/3	NONE/PRINT/AUXILIARY/BOTH REGION AVERAGED FLUX
0	IEDF(10)	0/1/2/3	NONE/PWDINT/RZFLUX/BOTH FILES TO BE WRITTEN
0	ISRHED	-1/0/N	NONE/INPUT-1ST PASS, OUTPUT-LAST SEARCH PASS/REQUESTED EDITS (ABOVE) EVERY N-TH SEARCH PASS

CONVERGENCE CRITERIA

1.0000000D-07	EPS1	DESIRED EIGENVALUE CONVERGENCE
1.0000000D-05	EPS2	DESIRED POINTWISE FISSION SOURCE CONVERGENCE
1.0000000D-05	EPS3	DESIRED AVERAGE FISSION SOURCE CONVERGENCE

OTHER FLOATING POINT DATA

1.0000000D+00	EPFK	K-EFFECTIVE OF REACTOR
1.0000000D-03	FISMIN	CUT-OFF POINT FOR CONSIDERATION OF A FISSION SOURCE IN CALCULATING FLAMUP AND FLAMLO
4.0000000D-02	PSIRRM	INNER ITERATION ERROR REDUCTION FACTOR PER OUTER ITERATION
5.0000000D-01	POWIN	STEADY STATE REACTOR POWER (WATTS)

*** PROBLEM DESCRIPTION ***

NO. OF FIRST DIMENSION MESH INTERVALS	= 31
NO. OF SECOND DIMENSION MESH INTERVALS	= 16
NO. OF THIRD DIMENSION MESH INTERVALS	= 1
NO. OF ZONES	= 6
NO. OF REGIONS	= 5
NO. OF ENERGY GROUPS	= 4
MAXIMUM NO. OF DOWNSCATTER GROUPS	= 3
MAXIMUM NO. OF UPSCATTER GROUPS	= 0

PROBLEM GEOMETRY - 2-DIMENSIONAL TRIANGULAR

RHOMBIC BOUNDARY WITH 60 DEGREE (SIXTH CORE) SYMMETRY

TRIANGLE SIDE LENGTH = 6.466496D+00

BOUNDARY CONDITIONS (ORIGIN AT LOWER LEFT)

0 - ZERO FLUX 1 - ZERO CURRENT 2 - EXTRAPOLATED 3 - PERIODIC OPPOSITE FACE
4 - PERIODIC NEXT ADJACENT FACE 5 - INVERTED PERIODIC A LONG FACE

X - LEFT	X - RIGHT	Y - FRONT	Y - BACK
4	2	4	2

BOUNDARY CONDITION 2 IS APPLIED TO MESH CELL SURFACES ADJACENT TO EXCLUDED BACKGROUND CELLS.

EXTRAPOLATED BOUNDARY CONDITION CONSTANTS C
(DEL PHI/PHI = C/D , LAST VALUE USED FOR REMAINING GROUPS

GROUP	TRIAG = 0.0	TRIAG = 0.0	= 0.0	= 0.0
1	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01
2	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01
3	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01
4	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01

INTERNAL BLACK BOUNDARY CONDITION CONSTANT C FOR ALL GROUPS
(DEL PHI/PHI = C/D

0.0

BUCKLING SPECIFICATION FOR ALL ZONE

BUCKLING = 0.0

REGION NUMBER AND ASSIGNMENT TO ZONE

REGION NO.	NAME	ZONE NO.	ZONE NAME	REGION NO.	NAME	ZONE NO.	ZONE NAME	REGION NO.	NAME	ZONE NO.	ZONE NAME	REGION NO.	NAME	ZONE NO.	ZONE NAME
1	IC	1	M1	2	OC	2	M2	3	RB	3	M3	4	CR	5	M5
5	CF	6	M6												

*** EDIT OF MACROSCOPIC CROSS SECTION DATASET COMPXS ***

NO. OF COMPOSITIONS	=	6
NO. OF PRECURSOR FAMILIES	=	0
NO. OF ENERGY GROUPS	=	4
MAXIMUM NO. OF DOWNSCATTER GROUPS	=	3
MAXIMUM NO. OF UPSCATTER GROUPS	=	0
MAXIMUM ENERGY BOUND (EV)	=	1.05000D+07
MINIMUM ENERGY BOUND (EV)	=	0.0

GROUP NO.	NEUTRON VELOCITY (CM/SEC)	MAXIMUM ENERGY (EV)	MAX DOWNSCATTER	MAX UPSCATTER
1	1.7233600D+09	1.0500000D+07	0	0
2	4.0246298D+08	8.0000000D+05	1	0
3	7.9700304D+07	1.0000000D+04	2	0
4	3.1594608D+07	1.0000000D+03	3	0

********** EDIT OF FISSIONABLE COMPOSITION 1 (M1) IN COMPXS **********

GROUP	ABSORPTION CROSS SECTION	DIRECTIONAL DIFFUSION COEFFICIENTS D1	D2	D3	REMOVAL CROSS SECTION	FISSION CROSS SECTION	FISSION SPECTRUM(CHI)	NEUTRONS PER FISSION	POWER CONVER. FACTOR
1	4.602890D-03	2.876787D+00	2.876787D+00	2.876787D+00	2.820400D-02	3.912300D-03	7.680000D-01	3.036066D+00	1.262032D-13
2	3.659358D-03	1.570845D+00	1.570845D+00	1.570845D+00	5.274700D-03	1.828600D-03	2.320000D-01	2.912173D+00	5.898711D-14
3	1.292820D-02	7.224859D-01	7.224859D-01	7.224859D-01	1.761200D-02	3.633400D-03	0.0	2.881874D+00	1.172065D-13
4	2.654650D-02	9.641993D-01	9.641993D-01	9.641993D-01	2.654650D-02	9.241499D-03	0.0	2.879511D+00	2.981129D-13

SCATTERING CROSS SECTION (TOTAL)

INTO GROUP	FROM GROUP					
2	1	2.359700D-02				
3	1	4.079100D-06	2	1.615300D-03		
4	1	4.449300D-08	2	4.230900D-08	3	4.683800D-03

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.100 PAGE 23

********** EDIT OF FISSIONABLE COMPOSITION 2 (M2) IN COMPXS **********

GROUP	ABSORPTION CROSS SECTION	DIRECTIONAL DIFFUSION COEFFICIENTS D1	D2	D3	REMOVAL CROSS SECTION	FISSION CROSS SECTION	FISSION SPECTRUM(CHI)	NEUTRONS PER FISSION	POWER CONVER. FACTOR
1	5.515310D-03	2.876539D+00	2.876539D+00	2.876539D+00	2.878200D-02	4.853100D-03	7.680000D-01	3.079063D+00	1.565516D-13
2	4.477260D-03	1.571363D+00	1.571363D+00	1.571363D+00	6.049101D-03	2.637700D-03	2.320000D-01	2.914926D+00	8.508711D-14
3	1.516860D-02	7.127076D-01	7.127076D-01	7.127076D-01	1.951000D-02	5.133200D-03	0.0	2.884945D+00	1.655871D-13
4	3.371400D-02	9.429781D-01	9.429781D-01	9.429781D-01	3.371400D-02	1.323800D-02	0.0	2.882535D+00	4.270324D-13

SCATTERING CROSS SECTION (TOTAL)

INTO GROUP	FROM GROUP					
2	1	2.326200D-02				
3	1	4.645100D-06	2	1.571800D-03		
4	1	4.996800D-08	2	4.072400D-08	3	4.341401D-03

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.100 PAGE 24

********** EDIT OF FISSIONABLE COMPOSITION 3 (M3) IN COMPXS **********

GROUP	ABSORPTION CROSS SECTION	DIRECTIONAL DIFFUSION COEFFICIENTS D1	D2	D3	REMOVAL CROSS SECTION	FISSION CROSS SECTION	FISSION SPECTRUM(CHI)	NEUTRONS PER FISSION	POWER CONVER. FACTOR
1	3.884070D-03	2.285610D+00	2.285610D+00	2.285610D+00	3.595900D-02	2.768800D-03	7.680000D-01	2.796410D+00	8.931614D-14
2	3.107810D-03	1.171934D+00	1.171934D+00	1.171934D+00	5.885500D-03	4.434701D-05	2.320000D-01	2.440977D+00	1.430549D-15
3	1.014390D-02	6.324751D-01	6.324751D-01	6.324751D-01	1.604100D-02	1.227400D-04	0.0	2.423171D+00	3.959356D-15
4	1.334902D-02	8.183573D-01	8.183573D-01	8.183573D-01	1.334902D-02	3.495200D-04	0.0	2.422951D+00	1.127484D-14

SCATTERING CROSS SECTION (TOTAL)

INTO GROUP	FROM GROUP					
2	1	3.207100D-02				
3	1	3.888000D-06	2	2.777600D-03		
4	1	4.503900D-08	2	9.001798D-08	3	5.897101D-03

********** EDIT OF FISSIONABLE COMPOSITION 4 (M4) IN COMPXS **********

GROUP	ABSORPTION CROSS SECTION	DIRECTIONAL DIFFUSION COEFFICIENTS D1	D2	D3	REMOVAL CROSS SECTION	FISSION CROSS SECTION	FISSION SPECTRUM(CHI)	NEUTRONS PER FISSION	POWER CONVER. FACTOR
1	2.768080D-03	2.716654D+00	2.716654D+00	2.716654D+00	2.909300D-02	1.945300D-03	7.680000D-01	2.790264D+00	6.275163D-14
2	2.201938D-03	1.440943D+00	1.440943D+00	1.440943D+00	4.490900D-03	3.106501D-05	2.320000D-01	2.441880D+00	1.002097D-15
3	7.728397D-03	7.203469D-01	7.203469D-01	7.203469D-01	1.308200D-02	8.756600D-05	0.0	2.423086D+00	2.824710D-15
4	9.956190D-03	9.876835D-01	9.876835D-01	9.876835D-01	9.956190D-03	2.376900D-04	0.0	2.422988D+00	7.667421D-15

SCATTERING CROSS SECTION (TOTAL)

INTO GROUP	FROM GROUP					
2	1	2.632200D-02				
3	1	2.890700D-06	2	2.288900D-03		
4	1	3.324800D-08	2	6.213298D-08	3	5.353600D-03

********** EDIT OF NON-FISSIONABLE COMPOSITION 5 (M5) IN COMPXS **********

GROUP	ABSORPTION CROSS SECTION	DIRECTIONAL DIFFUSION COEFFICIENTS D1	D2	D3	REMOVAL CROSS SECTION	POWER CONVERSION FACTOR
1	1.866960D-03	2.503066D+00	2.503066D+00	2.503066D+00	2.481400D-02	0.0
2	1.264330D-02	1.314665D+00	1.314665D+00	1.314665D+00	1.641200D-02	0.0
3	6.344050D-02	5.742770D-01	5.742770D-01	5.742770D-01	7.212200D-02	0.0
4	1.686800D-01	6.153695D-01	6.153695D-01	6.153695D-01	1.686800D-01	0.0

SCATTERING CROSS SECTION (TOTAL)

INTO GROUP	FROM GROUP					
2	1	2.294600D-02				
3	1	1.032000D-06	2	3.768700D-03		
4	1	1.048900D-08	2	7.036100D-12	3	8.681498D-03

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.100 PAGE 27

********** EDIT OF NON-FISSIONABLE COMPOSITION 6 (M6) IN COMPXS **********

GROUP	ABSORPTION CROSS SECTION	DIRECTIONAL DIFFUSION COEFFICIENTS D1	D2	D3	REMOVAL CROSS SECTION	POWER CONVERSION FACTOR
1	2.163050D-04	4.616420D+00	4.616420D+00	4.616420D+00	1.315900D-02	0.0
2	1.688000D-04	2.901831D+00	2.901831D+00	2.901831D+00	1.455900D-03	0.0
3	1.146800D-03	1.021179D+00	1.021179D+00	1.021179D+00	4.600100D-03	0.0
4	7.865999D-04	1.729625D+00	1.729625D+00	1.729625D+00	7.865999D-04	0.0

SCATTERING CROSS SECTION (TOTAL)

INTO GROUP	FROM GROUP					
2	1	1.294200D-02				
3	1	6.878000D-07	2	1.287100D-03		
4	1	6.990302D-09	2	4.363300D-12	3	3.453300D-03

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.100 PAGE 28

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS
1	1.42092D+00	7	2	1.57656D+00	11	3	1.27169D+00	5	4	1.26615D+00	5

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
1	6.055469D-01	1.686693D-01	5.676263D-02	0	0.0	0.0	1.05676263D+00
2	4.704232D-01	1.306399D-01	3.391310D-02	0	0.0	8.269922D-01	1.09067574D+00
3	1.767146D-01	7.337978D-02	1.908419D-02	0	0.0	5.957153D-01	1.10975993D+00
4	8.690130D-02	4.552007D-02	8.680460D-03	1	5.957153D-01	5.957153D-01	1.11844039D+00
5	3.722962D-02	2.073863D-02	5.107754D-03	2	5.957153D-01	6.254009D-01	1.12354814D+00
6	1.064050D-02	6.314254D-03	2.468417D-03	3	5.957153D-01	6.280142D-01	1.12601656D+00
7	3.829818D-03	2.197660D-03	8.781398D-04	1	6.280142D-01	6.280142D-01	1.12689470D+00
8	1.806451D-03	1.012883D-03	2.399321D-04	2	6.280142D-01	6.305913D-01	1.12713463D+00
9	4.606560D-04	2.320342D-04	9.278793D-05	3	6.280142D-01	6.203958D-01	1.12722742D+00
10	1.203257D-04	7.173725D-05	3.893697D-05	4	6.280142D-01	6.331385D-01	1.12726635D+00
11	2.823481D-05	1.472779D-05	1.050205D-05	1	6.331385D-01	6.331385D-01	1.12727686D+00
12	1.556538D-05	1.031790D-05	2.427902D-06	2	6.331385D-01	7.953652D-01	1.12727928D+00
13	4.066891D-06	1.710762D-06	7.286502D-07	3	6.331385D-01	6.304855D-01	1.12728001D+00
14	9.684399D-07	7.739674D-07	3.097159D-07	4	6.331385D-01	6.577679D-01	1.12728032D+00
15	2.049522D-07	1.272518D-07	8.601389D-08	1	6.577679D-01	6.577679D-01	1.12728041D+00

OUTER ITERATIONS COMPLETED AT ITERATION 15, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.12728040833

TO RESTART THIS CALCULATION, INPUT FOLLOWING VALUES

DOMINANCE RATIO (SIGBAR) = 6.577679231397D-01

OPTIMIZED OVER-RELAXATION FACTORS

GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA
1	1.42092D+00	2	1.57656D+00	3	1.27169D+00	4	1.26615D+00		

MAXIMUM POWER DENSITY 2.68379D-04 OCCURS AT MESH CELL (I,J,K) = (1, 1, 1)

PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX VALUES ON THE CELL SURFACES AND WITHIN THE CELL.

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.200 PAGE 29

REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0,1.050D+07)

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	IC	1	M1	1.43043D+03	1.00000D+00	2.86439D-01	2.00247D-04	2.68379D-04	1.34024D+00	5.72878D-01
2	OC	2	M2	1.52096D+03	1.00000D+00	2.04546D-01	1.34485D-04	2.26994D-04	1.68788D+00	4.09092D-01
3	RB	3	M3	1.95552D+03	1.00000D+00	9.01489D-03	4.60997D-06	1.81598D-05	3.93925D+00	1.80298D-02
4	CR	5	M5	2.17280D+02	1.00000D+00	0.0	0.0	0.0	0.0	0.0
5	CF	6	M6	1.08640D+02	1.00000D+00	0.0	0.0	0.0	0.0	0.0
	TOTALS			5.23283D+03	0.0	5.00000D-01	9.55506D-05	2.68379D-04	2.80876D+00	1.00000D+00

AREA NO.	AREA NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	TCORE	2.95139D+03	0.0	4.90985D-01	1.66357D-04	2.68379D-04	1.61327D+00	9.81970D-01
2	TROD	3.25920D+02	0.0	0.0	0.0	0.0	0.0	0.0
3	TOTAL	5.23283D+03	0.0	5.00000D-01	9.55506D-05	2.68379D-04	2.80876D+00	1.00000D+00

(1) INTEGRATION WEIGHT FACTOR = (2/B)*SIN(B*H) H=UNEXTRAPOLATED HALF HEIGHT, B=BUCKLING COEFFICIENT
(2) THE PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX ON THE CELL SURFACES AND WITHIN THE CELL.

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	IC	1	M1	1.00000D+00	1.00000D+00	1.00000D+00
2	OC	2	M2	1.00000D+01	5.00000D+00	1.00000D+00
3	RB	3	M3	1.40000D+01	7.00000D+00	1.00000D+00
4	CR	5	M5	0.0	0.0	0.0
5	CF	6	M6	0.0	0.0	0.0
	TOTALS			1.00000D+00	1.00000D+00	1.00000D+00

AREA NO.	AREA NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	TCORE	1.00000D+00	1.00000D+00	1.00000D+00
2	TROD	0.0	0.0	0.0
3	TOTAL	1.00000D+00	1.00000D+00	1.00000D+00

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.200 PAGE 30

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(8.000D+05,1.050D+07) FOR GROUP 1

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	IC	1	M1	1.57665D+09	2.64407D+09	1.35573D+10	0.0	1.77781D+10	0.0	-9.77753D+02
2	OC	2	M2	3.27070D+09	1.81707D+09	7.66543D+09	0.0	1.27532D+10	0.0	1.63776D+03
3	RB	3	M3	-2.51636D+09	3.28094D+08	2.70943D+09	0.0	5.21158D+08	0.0	1.02278D+02
4	CR	5	M5	-1.28618D+09	9.67696D+07	1.18941D+09	0.0	0.0	0.0	-6.99544D-01
5	CF	6	M6	-5.62052D+08	9.23891D+06	5.52814D+08	0.0	0.0	0.0	-3.63760D+00
	TOTALS			4.82764D+08	4.89524D+09	2.56744D+10	0.0	3.10524D+10	0.0	7.57947D+02

AREA NO.	AREA NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	TCORE	4.84735D+09	4.46114D+09	2.12228D+10	0.0	3.05313D+10	0.0	6.60006D+02
2	TROD	-1.84823D+09	1.06009D+08	1.74222D+09	0.0	0.0	0.0	-4.33714D+00
3	TOTAL	4.82764D+08	4.89524D+09	2.56744D+10	0.0	3.10524D+10	0.0	7.57947D+02

(1) ABSORPTION = CAPTURE + FISSION
(2) SCATTER OUT = TOTAL OUTSCATTER - (N,2N) SOURCE
(3) FISSION PRODUCTION = FISSION SOURCE / K-EFF

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	IC	1	M1	1.57665D+09	4.06954D+08	0.0	9.54084D-04	9.54084D-04	2.46261D-04	0.0
2	OC	2	M2	3.27070D+09	8.03841D+08	0.0	3.45119D-03	3.45119D-03	8.48200D-04	0.0
3	RB	3	M3	-2.51636D+09	-4.82004D+08	0.0	-1.30334D-02	-1.30334D-02	-2.49653D-03	0.0
4	CR	5	M5	-1.28618D+09	-4.48257D+08	0.0	-9.91344D-03	-9.91344D-03	-3.45502D-03	0.0
5	CF	6	M6	-5.62052D+08	-1.77414D+08	0.0	-2.85048D-03	-2.85048D-03	-8.99762D-04	0.0
	TOTALS			4.82764D+08	1.03121D+08	0.0	1.54721D-04	1.54721D-04	3.30493D-05	0.0

AREA NO.	AREA NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	TCORE	4.84735D+09	1.21080D+09	0.0	1.86420D-03	1.86420D-03	4.65649D-04	0.0
2	TROD	-1.84823D+09	-6.25670D+08	0.0	-5.65348D-03	-5.65348D-03	-1.91384D-03	0.0
3	TOTAL	4.82764D+08	1.03121D+08	0.0	1.54721D-04	1.54721D-04	3.30493D-05	0.0

(4) BUCKLING = B**2 = LEAKAGE / (D*FLUX*VOLUME) 1/CM**2

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 31

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(8.000D+05,1.050D+07) FOR GROUP 1

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	CAPTURE RATE	FISSION RATE
1	IC	1	M1	3.96700D+08	2.24737D+09
2	OC	2	M2	2.18171D+08	1.59890D+09
3	RB	3	M3	9.42088D+07	2.33885D+08
4	CR	5	M5	9.67696D+07	0.0
5	CF	6	M6	9.23891D+06	0.0
	TOTALS			8.15089D+08	4.08015D+09

AREA NO.	AREA NAME	CAPTURE RATE	FISSION RATE
1	TCORE	6.14871D+08	3.84627D+09
2	TROD	1.06009D+08	0.0
3	TOTAL	8.15089D+08	4.08015D+09

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 32

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(1.000D+04,8.000D+05) FOR GROUP 2

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	IC	1	M1	3.74742D+09	1.05298D+10	4.64816D+09	1.35550D+10	5.37046D+09	0.0	-4.34370D+02
2	OC	2	M2	2.62129D+09	6.58375D+09	2.31137D+09	7.66388D+09	3.85253D+09	0.0	4.53192D+02
3	RB	3	M3	-7.60597D+08	1.91529D+09	1.71184D+09	2.70909D+09	1.57433D+08	0.0	2.75525D+01
4	CR	5	M5	-2.71777D+09	3.00993D+09	8.97197D+08	1.18935D+09	0.0	0.0	-3.16520D+00
5	CF	6	M6	2.12795D+08	3.94190D+07	3.00570D+08	5.52784D+08	0.0	0.0	-1.69340D+01
	TOTALS			3.10313D+09	2.20782D+10	9.86914D+09	2.56701D+10	9.38042D+09	0.0	2.62747D+01

AREA NO.	AREA NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	TCORE	6.36871D+09	1.71136D+10	6.95954D+09	2.12189D+10	9.22298D+09	0.0	1.88213D+01
2	TROD	-2.50498D+09	3.04935D+09	1.19777D+09	1.74214D+09	0.0	0.0	-2.00992D+01
3	TOTAL	3.10313D+09	2.20782D+10	9.86914D+09	2.56701D+10	9.38042D+09	0.0	2.62747D+01

(1) ABSORPTION = CAPTURE + FISSION
(2) SCATTER OUT = TOTAL OUTSCATTER - (N,2N) SOURCE
(3) FISSION PRODUCTION = FISSION SOURCE / K-EFF

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	IC	1	M1	3.74742D+09	8.49477D+08	0.0	8.29053D-04	8.29053D-04	1.87932D-04	0.0
2	OC	2	M2	2.62129D+09	5.90552D+08	0.0	1.13443D-03	1.13443D-03	2.55576D-04	0.0
3	RB	3	M3	-7.60597D+08	2.79571D+07	0.0	-1.05311D-03	-1.05311D-03	3.87088D-05	0.0
4	CR	5	M5	-2.71777D+09	-8.74492D+08	0.0	-8.68365D-03	-8.68365D-03	-2.79412D-03	0.0
5	CF	6	M6	2.12795D+08	8.81135D+07	0.0	3.14020D-04	3.14020D-04	1.30028D-04	0.0
	TOTALS			3.10313D+09	6.81608D+08	0.0	3.63209D-04	3.63209D-04	7.97793D-05	0.0

AREA NO.	AREA NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	TCORE	6.36871D+09	1.44003D+09	0.0	9.32353D-04	9.32353D-04	2.10814D-04	0.0
2	TROD	-2.50498D+09	-7.86378D+08	0.0	-2.52868D-03	-2.52868D-03	-7.93820D-04	0.0
3	TOTAL	3.10313D+09	6.81608D+08	0.0	3.63209D-04	3.63209D-04	7.97793D-05	0.0

(4) BUCKLING = B**2 = LEAKAGE / (D*FLUX*VOLUME) 1/CM**2

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 33

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(1.000D+04,8.000D+05) FOR GROUP 2

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	CAPTURE RATE	FISSION RATE
1	IC	1	M1	5.26803D+09	5.26182D+09
2	OC	2	M2	2.70505D+09	3.87870D+09
3	RB	3	M3	1.88795D+09	2.73302D+07
4	CR	5	M5	3.00993D+09	0.0
5	CF	6	M6	3.94190D+07	0.0
	TOTALS			1.29104D+10	9.16785D+09

AREA NO.	AREA NAME	CAPTURE RATE	FISSION RATE
1	TCORE	7.97308D+09	9.14052D+09
2	TROD	3.04935D+09	0.0
3	TOTAL	1.29104D+10	9.16785D+09

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 34

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(1.000D+03,1.000D+04) FOR GROUP 3

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	IC	1	M1	6.45877D+07	3.36623D+09	1.21956D+09	4.65039D+09	0.0	0.0	-7.18331D+01
2	OC	2	M2	-6.58282D+07	1.84936D+09	5.29306D+08	2.31284D+09	0.0	0.0	9.56224D+00
3	RB	3	M3	3.63142D+08	8.53052D+08	4.95917D+08	1.71211D+09	0.0	0.0	1.71880D+00
4	CR	5	M5	-2.41728D+08	1.00188D+09	1.37102D+08	8.97250D+08	0.0	0.0	6.93582D-01
5	CF	6	M6	1.84679D+08	2.88988D+07	8.70215D+07	3.00599D+08	0.0	0.0	-6.75876D+00
	TOTALS			3.04852D+08	7.09943D+09	2.46891D+09	9.87319D+09	0.0	0.0	-6.66173D+01

AREA NO.	AREA NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	TCORE	-1.24053D+06	5.21560D+09	1.74887D+09	6.96323D+09	0.0	0.0	-6.22709D+01
2	TROD	-5.70492D+07	1.03078D+09	2.24123D+08	1.19785D+09	0.0	0.0	-6.06518D+00
3	TOTAL	3.04852D+08	7.09943D+09	2.46891D+09	9.87319D+09	0.0	0.0	-6.66173D+01

(1) ABSORPTION = CAPTURE + FISSION
(2) SCATTER OUT = TOTAL OUTSCATTER - (N,2N) SOURCE
(3) FISSION PRODUCTION = FISSION SOURCE / K-EFF

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	IC	1	M1	6.45877D+07	-1.34218D+06	0.0	3.43332D-04	3.43332D-04	-7.13467D-06	0.0
2	OC	2	M2	-6.58282D+07	-7.24701D+06	0.0	-7.57571D-04	-7.57571D-04	-8.34009D-05	0.0
3	RB	3	M3	3.63142D+08	9.08582D+07	0.0	6.82751D-03	6.82751D-03	1.70824D-03	0.0
4	CR	5	M5	-2.41728D+08	-7.65302D+07	0.0	-2.66537D-02	-2.66537D-02	-8.43847D-03	0.0
5	CF	6	M6	1.84679D+08	6.19366D+07	0.0	7.17668D-03	7.17668D-03	2.40687D-03	0.0
	TOTALS			3.04852D+08	6.76754D+07	0.0	8.39803D-04	8.39803D-04	1.86431D-04	0.0

AREA NO.	AREA NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	TCORE	-1.24053D+06	-8.58919D+06	0.0	-4.51077D-06	-4.51077D-06	-3.12318D-05	0.0
2	TROD	-5.70492D+07	-1.45936D+07	0.0	-1.63923D-03	-1.63923D-03	-4.19328D-04	0.0
3	TOTAL	3.04852D+08	6.76754D+07	0.0	8.39803D-04	8.39803D-04	1.86431D-04	0.0

(4) BUCKLING = B**2 = LEAKAGE / (D*FLUX*VOLUME) 1/CM**2

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 35

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(1.000D+03,1.000D+04) FOR GROUP 3

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	CAPTURE RATE	FISSION RATE
1	IC	1	M1	2.42017D+09	9.46062D+08
2	OC	2	M2	1.22352D+09	6.25843D+08
3	RB	3	M3	8.42730D+08	1.03218D+07
4	CR	5	M5	1.00188D+09	0.0
5	CF	6	M6	2.88988D+07	0.0
	TOTALS			5.51720D+09	1.58223D+09

AREA NO.	AREA NAME	CAPTURE RATE	FISSION RATE
1	TCORE	3.64369D+09	1.57190D+09
2	TROD	1.03078D+09	0.0
3	TOTAL	5.51720D+09	1.58223D+09

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 36

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.000D+03) FOR GROUP 4

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	IC	1	M1	7.11501D+05	1.21900D+09	0.0	1.21971D+09	0.0	0.0	-1.95035D+01
2	OC	2	M2	-7.54205D+07	6.04803D+08	0.0	5.29383D+08	0.0	0.0	3.47536D+00
3	RB	3	M3	1.93332D+08	3.02644D+08	0.0	4.95977D+08	0.0	0.0	2.38160D+00
4	CR	5	M5	-8.69602D+07	2.24062D+08	0.0	1.37102D+08	0.0	0.0	1.01616D-01
5	CF	6	M6	8.29646D+07	4.05718D+06	0.0	8.70218D+07	0.0	0.0	-2.94183D+00
	TOTALS			1.14628D+08	2.35457D+09	0.0	2.46919D+09	0.0	0.0	-1.64868D+01

AREA NO.	AREA NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	TCORE	-7.47090D+07	1.82380D+09	0.0	1.74909D+09	0.0	0.0	-1.60282D+01
2	TROD	-3.99564D+06	2.28120D+08	0.0	2.24124D+08	0.0	0.0	-2.84021D+00
3	TOTAL	1.14628D+08	2.35457D+09	0.0	2.46919D+09	0.0	0.0	-1.64868D+01

(1) ABSORPTION = CAPTURE + FISSION
(2) SCATTER OUT = TOTAL OUTSCATTER - (N,2N) SOURCE
(3) FISSION PRODUCTION = FISSION SOURCE / K-EFF

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	IC	1	M1	7.11501D+05	-6.94211D+06	0.0	1.60699D-05	1.60699D-05	-1.56794D-04	0.0
2	OC	2	M2	-7.54205D+07	-1.26134D+07	0.0	-4.45845D-03	-4.45845D-03	-7.45634D-04	0.0
3	RB	3	M3	1.93332D+08	4.50569D+07	0.0	1.04203D-02	1.04203D-02	2.42849D-03	0.0
4	CR	5	M5	-8.69602D+07	-2.72170D+07	0.0	-1.06385D-01	-1.06385D-01	-3.32965D-02	0.0
5	CF	6	M6	8.29646D+07	2.76208D+07	0.0	9.29974D-03	9.29974D-03	3.09609D-03	0.0
	TOTALS			1.14628D+08	2.59053D+07	0.0	1.28099D-03	1.28099D-03	2.89496D-04	0.0

AREA NO.	AREA NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	TCORE	-7.47090D+07	-1.95555D+07	0.0	-1.22090D-03	-1.22090D-03	-3.19577D-04	0.0
2	TROD	-3.99564D+06	4.03804D+05	0.0	-4.10290D-04	-4.10290D-04	4.14643D-05	0.0
3	TOTAL	1.14628D+08	2.59053D+07	0.0	1.28099D-03	1.28099D-03	2.89496D-04	0.0

(4) BUCKLING = B**2 = LEAKAGE / (D*FLUX*VOLUME) 1/CM**2

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 37

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0,1.000D+03) FOR GROUP 4

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	CAPTURE RATE	FISSION RATE
1	IC	1	M1	7.94636D+08	4.24364D+08
2	OC	2	M2	3.67324D+08	2.37479D+08
3	RB	3	M3	2.94720D+08	7.92419D+06
4	CR	5	M5	2.24062D+08	0.0
5	CF	6	M6	4.05718D+06	0.0
	TOTALS			1.68480D+09	6.69768D+08

AREA NO.	AREA NAME	CAPTURE RATE	FISSION RATE
1	TCORE	1.16196D+09	6.61844D+08
2	TROD	2.28120D+08	0.0
3	TOTAL	1.68480D+09	6.69768D+08

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 38

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	IC	1	M1	5.38937D+09	1.77591D+10	1.94251D+10	1.94251D+10	2.31485D+10	0.0	-1.50346D+03
2	OC	2	M2	5.75074D+09	1.08550D+10	1.05061D+10	1.05061D+10	1.66057D+10	0.0	2.10399D+03
3	RB	3	M3	-2.72048D+09	3.39908D+09	4.91718D+09	4.91718D+09	6.78592D+08	0.0	1.33931D+02
4	CR	5	M5	-4.33264D+09	4.33264D+09	2.22371D+09	2.22371D+09	0.0	0.0	-3.06955D+00
5	CF	6	M6	-8.16137D+07	8.16139D+07	9.40405D+08	9.40405D+08	0.0	0.0	-3.02721D+01
	TOTALS			4.00538D+09	3.64275D+10	3.80125D+10	3.80125D+10	4.04328D+10	0.0	7.01118D+02

AREA NO.	AREA NAME	NET LEAKAGE +	ABSORPTION RATE(1) +	SCATTER OUT(2) -	SCATTER IN -	FISSION PRODUCTION(3) -	EXTERNAL SOURCE =	BALANCE
1	TCORE	1.11401D+10	2.86141D+10	2.99312D+10	2.99312D+10	3.97542D+10	0.0	6.00528D+02
2	TROD	-4.41425D+09	4.41425D+09	3.16411D+09	3.16411D+09	0.0	0.0	-3.33417D+01
3	TOTAL	4.00538D+09	3.64275D+10	3.80125D+10	3.80125D+10	4.04328D+10	0.0	7.01118D+02

(1) ABSORPTION = CAPTURE + FISSION
(2) SCATTER OUT = TOTAL OUTSCATTER - (N,2N) SOURCE (N,2N) SOURCE = SCATTER IN - SCATTER OUT
(3) FISSION PRODUCTION = FISSION SOURCE / K-EFF

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	IC	1	M1	5.38937D+09	1.24815D+09	0.0	8.41426D-04	8.41426D-04	1.94869D-04	0.0
2	OC	2	M2	5.75074D+09	1.37453D+09	0.0	1.71042D-03	1.71042D-03	4.08821D-04	0.0
3	RB	3	M3	-2.72048D+09	-3.18132D+08	0.0	-2.75617D-03	-2.75617D-03	-3.22305D-04	0.0
4	CR	5	M5	-4.33264D+09	-1.42650D+09	0.0	-9.57270D-03	-9.57270D-03	-3.15176D-03	0.0
5	CF	6	M6	-8.16137D+07	2.57230D+05	0.0	-8.97364D-05	-8.97364D-05		
2.82831D-07	0.0									
	TOTALS			4.00538D+09	8.78309D+08	0.0	3.30576D-04	3.30576D-04	7.24895D-05	0.0

AREA NO.	AREA NAME	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	TCORE	1.11401D+10	2.62268D+09	0.0	1.14056D-03	1.14056D-03	2.68518D-04	0.0
2	TROD	-4.41425D+09	-1.42624D+09	0.0	-3.24080D-03	-3.24080D-03	-1.04710D-03	0.0
3	TOTAL	4.00538D+09	8.78309D+08	0.0	3.30576D-04	3.30576D-04	7.24895D-05	0.0

(4) BUCKLING = B**2 = LEAKAGE / (D*FLUX*VOLUME) 1/CM**2

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 39

REGION AND AREA BALANCE INTEGRALS FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	CAPTURE RATE	FISSION RATE	(N2,N) SOURCE	NET PRODUCTION(5)	MEDIAN ENERGY FISSION SRC.	MEDIAN ENERGY ABSORPTN RATE	MEDIAN ENERGY FLUX
1	IC	1	M1	8.87953D+09	8.87961D+09	4.58523D+03	2.31485D+10	1.96454D+06	5.97212D+04	1.09702D+05
2	OC	2	M2	4.51407D+09	6.34093D+09	1.93424D+03	1.66057D+10	1.96454D+06	7.23545D+04	1.18641D+05
3	RB	3	M3	3.11961D+09	2.79462D+08	3.30957D+02	6.78592D+08	1.96454D+06	3.47039D+04	8.26269D+04
4	CR	5	M5	4.33264D+09	0.0	1.64067D+02	1.64067D+02	0.0	3.93165D+04	1.23109D+05
5	CF	6	M6	8.16139D+07	0.0	2.40705D+02	2.40705D+02	0.0	2.39350D+04	1.00436D+05
	TOTALS			2.09275D+10	1.55000D+10	7.25520D+03	4.04328D+10	1.96454D+06	5.68942D+04	1.08645D+05

AREA NO.	AREA NAME	CAPTURE RATE	FISSION RATE	(N2,N) SOURCE	NET PRODUCTION(5)	MEDIAN ENERGY FISSION SRC.	MEDIAN ENERGY ABSORPTN RATE	MEDIAN ENERGY FLUX
1	TCORE	1.33936D+10	1.52205D+10	6.51947D+03	3.97542D+10	1.96454D+06	6.42968D+04	1.12647D+05
2	TROD	4.41425D+09	0.0	4.04772D+02	4.04772D+02	0.0	3.90651D+04	1.11305D+05
3	TOTAL	2.09275D+10	1.55000D+10	7.25520D+03	4.04328D+10	1.96454D+06	5.68942D+04	1.08645D+05

(5) NET PRODUCTION = FISSION PRODUCTION + (N,2N) SOURCE

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 40

BALANCE INTEGRAL TOTALS BY GROUP FOR REAL K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

GROUP NO.	EMIN (EV)	EMAX (EV)	NET LEAKAGE	+ ABSORPTION RATE(1)	+ SCATTER OUT(2)	- SCATTER IN	- FISSION PRODUCTION(3)	- EXTERNAL SOURCE	= BALANCE
1	8.00D+05	1.05D+07	4.82764D+08	4.89524D+09	2.56744D+10	0.0	3.10524D+10	0.0	7.57947D+02
2	1.00D+04	8.00D+05	3.10313D+09	2.20782D+10	9.86914D+09	2.56701D+10	9.38042D+09		
0.0		2.62747D+01							
3	1.00D+03	1.00D+04	3.04852D+08	7.09943D+09	2.46891D+09	9.87319D+09	0.0	0.0	-6.66173D+01
4	0.0	1.00D+03	1.14628D+08	2.35457D+09	0.0	2.46919D+09	0.0	0.0	-1.64868D+01
	TOTALS		4.00538D+09	3.64275D+10	3.80125D+10	3.80125D+10	4.04328D+10	0.0	7.01118D+02

(1) ABSORPTION = CAPTURE + FISSION
(2) SCATTER OUT = TOTAL OUTSCATTER - (N,2N) SOURCE
(3) FISSION PRODUCTION = FISSION SOURCE / K-EFF

GROUP NO.	EMIN (EV)	EMAX (EV)	LEAKAGE PLANAR	LEAKAGE Y	LEAKAGE D*(B**2)	BUCKLING(4) TOTAL	BUCKLING(4) PLANAR	BUCKLING(4) Y	BUCKLING(4) Z
1	8.00D+05	1.05D+07	4.82764D+08	1.03121D+08	0.0	1.54721D-04	1.54721D-04	3.30493D-05	0.0
2	1.00D+04	8.00D+05	3.10313D+09	6.81608D+08	0.0	3.63209D-04	3.63209D-04	7.97793D-05	0.0
3	1.00D+03	1.00D+04	3.04852D+08	6.76754D+07	0.0	8.39803D-04	8.39803D-04	1.86431D-04	0.0
4	0.0	1.00D+03	1.14628D+08	2.59053D+07	0.0	1.28099D-03	1.28099D-03	2.89426D-04	0.0
	TOTALS		4.00538D+09	8.78309D+08	0.0	3.30576D-04	3.30576D-04	7.24895D-05	0.0

(4) BUCKLING = B**2 = LEAKAGE / (D*FLUX*VOLUME) 1/CM**2

GROUP NO.	EMIN (EV)	EMAX (EV)	CAPTURE RATE	FISSION RATE
1	8.00D+05	1.05D+07	8.15089D+08	4.08015D+09
2	1.00D+04	8.00D+05	1.29104D+10	9.16785D+09
3	1.00D+03	1.00D+04	5.51720D+09	1.58223D+09
4	0.0	1.00D+03	1.68480D+09	6.69768D+08
	TOTALS		2.09275D+10	1.55000D+10

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 41

REGION AND AREA REAL FLUX INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	TOTAL FLUX (NEUTRON-CM/SEC)	PEAK FLUX (1) (NEUTRON/CM2-SEC)	TOTAL FAST FLUX (NEUTRON-CM/SEC)	PEAK FAST FLUX(1) (NEUTRON/CM2-SEC)
1	IC	1	M1	1.43043D+03	3.75825D+12	3.52624D+09	1.93993D+12	1.82299D+09
2	OC	2	M2	1.52096D+03	1.93981D+12	2.14926D+09	1.02726D+12	1.12598D+09
3	RB	3	M3	1.95552D+03	8.07520D+11	1.20060D+09	3.76921D+11	6.14409D+08
4	CR	5	M5	2.17280D+02	3.07019D+11	1.72130D+09	1.64804D+11	9.09090D+08
5	CF	6	M6	1.08640D+02	3.06595D+11	2.96550D+09	1.53529D+11	1.49456D+09
	TOTALS			5.23283D+03	7.11919D+12	3.52624D+09	3.66244D+12	1.82299D+09

AREA NO.	AREA NAME	VOLUME (CC)	TOTAL FLUX (NEUTRON-CM/SEC)	PEAK FLUX (1) (NEUTRON/CM2-SEC)	TOTAL FAST FLUX (NEUTRON-CM/SEC)	PEAK FAST FLUX(1) (NEUTRON/CM2-SEC)
1	TCORE	2.95139D+03	5.69805D+12	3.52624D+09	2.96719D+12	1.82299D+09
2	TROD	3.25920D+02	6.13613D+11	2.96550D+09	3.18333D+11	1.49456D+09
3	TOTAL	5.23283D+03	7.11919D+12	3.52624D+09	3.66244D+12	1.82299D+09

(1) PEAK FLUX CALCULATIONS ARE COMPUTED BY SAMPLING AVERAGE FLUXES ON THE SURFACE AND WITHIN EACH MESH CELL.

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	GROUP 1	GROUP 2	GROUP 3	GROUP 4
1	IC	1	M1	5.74436D+11	2.87751D+12	2.60379D+11	4.59194D+10
2	OC	2	M2	3.29459D+11	1.47049D+12	1.21921D+11	1.79392D+10
3	RB	3	M3	8.44717D+10	6.16281D+11	8.40951D+10	2.26716D+10
4	CR	5	M5	5.18327D+10	2.38065D+11	1.57924D+10	1.32833D+09
5	CF	6	M6	4.27124D+10	2.33525D+11	2.51995D+10	5.15786D+09
	TOTALS			1.08291D+12	5.43587D+12	5.07387D+11	9.30165D+10

AREA NO.	AREA NAME	GROUP 1	GROUP 2	GROUP 3	GROUP 4
1	TCORE	9.03896D+11	4.34800D+12	3.82300D+11	6.38586D+10
2	TROD	9.45451D+10	4.71590D+11	4.09919D+10	6.48619D+09
3	TOTAL	1.08291D+12	5.43587D+12	5.07387D+11	9.30165D+10

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 1 **** 2D SNR BENCHMARK - RODS IN - FD06 1/05/84 2222.300 PAGE 42

REAL ZONE FLUX AVERAGES FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

ZONE NO.	ZONE NAME	VOLUME (CC)	AVG. TOTAL FLUX (NEUTRON/CM2-SEC)	GROUP 1	GROUP 2	GROUP 3	GROUP 4
1	M1	1.43043D+03	2.62736D+09	4.01584D+08	2.01164D+09	1.82029D+08	3.21019D+07
2	M2	1.52096D+03	1.27538D+09	2.16613D+08	9.66815D+08	8.01603D+07	1.17947D+07
3	M3	1.95552D+03	4.12944D+08	4.31965D+07	3.15149D+08	4.30039D+07	1.15937D+07
4	M4	0.0	0.0	0.0	0.0	0.0	0.0
5	M5	2.17280D+02	1.41301D+09	2.38553D+08	1.09566D+09	7.26822D+07	6.11344D+06
6	M6	1.08640D+02	2.82211D+09	3.93155D+08	2.14953D+09	2.31954D+08	4.74766D+07
	TOTALS	5.23283D+03	1.36049D+09	2.06946D+08	1.03880D+09	9.69622D+07	1.77756D+07

*** THE FOLLOWING BINARY FILES HAVE BEEN WRITTEN ***

FILE NAME	VERSION NO.	LOGICAL UNIT
RTFLUX	1	30
DIF3D	1	18

BPOINTER SPACE USED, FCM = 409 ECM = 5992 WORDS

COMPUTING TIME SUMMARY	CENTRAL PROCESSOR (SEC)	PERIPHERAL PROCESSOR (SEC)
BINARY FILE INPUT PROCESSING	0.10	0.0
INITIALIZATION AND INPUT EDITTING	0.20	0.0
STEADY STATE REAL FLUX CALCULATION	1.55	0.0
EDIT REAL CALCULATION OUTPUT	0.77	0.0
STEADY STATE ADJOINT FLUX CALCULATION	0.0	0.0
EDIT ADJOINT CALCULATION OUTPUT	0.0	0.0
NODAL MATHEMATICAL-ADJOINT CALCULATION	0.0	0.0
TOTAL FOR THIS STEP	2.65	0.0
TOTAL ELAPSED COMPUTING TIME (SEC)	4.89 +	0.0 = 4.89

G.2 Sample Problem 2 (selected pages)

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GNIP4C 11/83              **** SAMPLE PROBLEM 2 ****  2D SNR BENCHMARK - RODS IN - NODAL        1/05/84  2222.300  PAGE  44

     *** GNIP4C - GENERAL NEUTRONICS BCD INPUT PROCESSOR TO CREATE CCCC BINARY INTERFACE FILES  ***

                                   *** GNIP4C CONTROL PARAMETERS  ***

      10000     IMAING     NO. OF WORDS OF MAIN MEMORY REQUESTED
          0     IBULKG     NO. OF WORDS OF BULK MEMORY REQUESTED
          0     IPRNTG     BPOINTER TRACE AND DUMP CONTROL (0/1/2/3, NEITHER/DUMP/TRACE/BOTH)
          1     IGMEDT     GEOMETRY PROCESSING EDIT CONTROL (0/1/2/3, NO EDITS/PRINT EDITS/EDITS TO AUXILIARY FILE/BOTH)
          0     IMAPR      REGION MAP OPTION (0/1/2/3, NO MAP/PRINT MAP/MAP TO AUXILIARY FILE/BOTH)
          0     IMAPZ      ZONE (COMPOSITION) MAP OPTION (0/1/2/3, SEE IMAPR)

     ****************************** TRICOM WARNING  163 ******************************
     WHEN HEXAGONAL GEOMETRY (A.NIP3 TYPE 03 CARD GEOMETRY TYPE SENTINEL VALUES
     BETWEEN 110 AND 128) AND PERIODIC BOUNDARY CONDITIONS ARE SPECIFIED, GNIP4C MAY
     USE THE PERIODICITY TO ASSIGN HEXES NOT REFERENCED ON TYPE 30 CARDS TO
     APPROPRIATE REGIONS.  THIS IS DONE SO THAT TYPE 30 CARDS COMPOSED FOR TRIANGULAR
     MESH MODELS CAN ALSO BE USED FOR HEXAGONAL MESH MODELS.  DIFFERENT SETS OF HEXES
     COMPRISE THE REGIONS OF SOLUTION IN TRIANGULAR AND HEXAGONAL GEOMETRIES.

                    CELL ( 6, 6) HAS BEEN ASSIGNED TO REGION OC
                    CELL ( 8, 8) HAS BEEN ASSIGNED TO REGION RB
                    CELL ( 9, 6) HAS BEEN ASSIGNED TO REGION OC
                    CELL (11, 7) HAS BEEN ASSIGNED TO REGION RB
                    CELL ( 7, 5) HAS BEEN ASSIGNED TO REGION CR
                    CELL ( 4, 4) HAS BEEN ASSIGNED TO REGION CF

     ********************************************************************************

                                   *** MODEL DESCRIPTION  ***

         10     IGOM       GEOMETRY TYPE, HEXAGONAL
          6     NZONE      NO. OF ZONES (COMPOSITIONS)
          5     NREG       NO. OF REGIONS
          1     NZCL       NO. OF ZONE CLASSIFICATIONS
         10     NCINTI     NO. OF 1ST DIMENSION COARSE MESH INTERVALS
         10     NCINTJ     NO. OF 2ND DIMENSION COARSE MESH INTERVALS
         10     NINTI      NO. OF 1ST DIMENSION FINE MESH INTERVALS
         10     NINTJ      NO. OF 2ND DIMENSION FINE MESH INTERVALS
          4     IMBI       FIRST BOUNDARY CONDITION, FIRST DIMENSION, PERIODIC, NEXT FACE CLOCKWISE
          2     IMB2       LAST BOUNDARY CONDITION, FIRST DIMENSION, EXTRAPOLATED
                JMBI       FIRST BOUNDARY CONDITION, SECOND DIMENSION, PERIODIC, SEE IMBI
          2     JMB2       LAST BOUNDARY CONDITION, SECOND DIMENSION, EXTRAPOLATED
          1     NBS        NO. OF BUCKLING SPECIFICATIONS
         24     NBCS       NO. OF CONSTANTS FOR EXTERNAL BOUNDARIES
          1     NIBCS      NO. OF CONSTANTS FOR INTERNAL BOUNDARIES
          0     NZWBB      NO. OF BLACKNESS THEORY ZONES
          0     NRASS      0/1, REGION ASSIGNMENTS TO COARSE/FINE MESH
          1     NTRIAG     OUTER BOUNDARY SHAPE, 60 DEGREE RHOMBUS
  1.1200D+01    FLAT       HEXAGON FLAT-TO-FLAT DISTANCE


GNIP4C 11/83              **** SAMPLE PROBLEM 2 ****  2D SNR BENCHMARK - RODS IN - NODAL        1/05/84  2222.300  PAGE  45

                  EXTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
                                LAST VALUE SHOWN IS USED FOR REMAINING GROUPS

LAST     HEX BOUNDARY

1 5.00000D-01    2 5.00000D-01    3 5.00000D-01    4 5.00000D-01

LAST          BOUNDARY

1 5.00000D-01    2 5.00000D-01    3 5.00000D-01    4 5.00000D-01


                                   REGION/ZONE SPECIFICATIONS

 REGION  REGION  REGION       ZONE  ZONE   ZONE
   NO.    NAME   VOLUME        NO.  NAME  CLASS.     BUCKLING BY GROUP (REPEAT LAST VALUE FOR REMAINING GROUPS)

     1    IC    1.430E+03      1   M1      0       0.0
     2    OC    1.521E+03      2   M2      0       0.0
     3    RB    1.956E+03      3   M3      0       0.0
     4    CR    2.173E+02      5   M5      0       0.0
     5    CF    1.086E+02      6   M6      0       0.0


                  INTERNAL BOUNDARY CONDITION CONSTANTS C (D * DEL PHI = - C * PHI), BY GROUP
                                LAST VALUE SHOWN IS USED FOR REMAINING GROUPS

1 0.0


                                   REGIONS COMPRISING AREAS

 AREA                REGION      REGION      REGION      REGION      REGION      REGION      REGION
 NO. NAME            NO. NAME    NO. NAME    NO. NAME    NO. NAME    NO. NAME    NO. NAME    NO. NAME

 1 TCORE             1 IC        2 OC
 2 TROD              4 CR        5 CF
 3 TOTAL             1 IC        2 OC        3 RB        4 CR        5 CF
```

*** PROBLEM DESCRIPTION ***

NO. OF FIRST DIMENSION MESH INTERVALS	= 10
NO. OF SECOND DIMENSION MESH INTERVALS	= 10
NO. OF THIRD DIMENSION MESH INTERVALS	= 1
NO. OF ZONES	= 6
NO. OF REGIONS	= 5
NO. OF ENERGY GROUPS	= 4
MAXIMUM NO. OF DOWNSCATTER GROUPS	= 3
MAXIMUM NO. OF UPSCATTER GROUPS	= 0

PROBLEM GEOMETRY - 2-DIMENSIONAL HEXAGONAL

BOUNDARY CONDITIONS (ORIGIN AT LOWER LEFT)

0 - ZERO FLUX 1 - ZERO CURRENT 2 - EXTRAPOLATED 3 - PERIODIC OPPOSITE FACE
4 - PERIODIC NEXT ADJACENT FACE 5 - INVERTED PERIODIC A LONG FACE

HEX = 0.0 HEX = 0.0 = 0.0 = 0.0

X - LEFT	X - RIGHT	Y - FRONT	Y - BACK
4	2	4	2

BOUNDARY CONDITION 2 IS APPLIED TO MESH CELL SURFACES ADJACENT TO EXCLUDED BACKGROUND CELLS.

EXTRAPOLATED BOUNDARY CONDITION CONSTANTS C
(DEL PHI/PHI = C/D , LAST VALUE USED FOR REMAINING GROUPS

GROUP	HEX = 0.0	HEX = 0.0	= 0.0	= 0.0
1	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01
2	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01
3	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01
4	4.692000D-01	4.999999D-01	4.692000D-01	4.999999D-01

INTERNAL BLACK BOUNDARY CONDITION CONSTANT C FOR ALL GROUPS
(DEL PHI/PHI = C/D

0.0

BUCKLING SPECIFICATION FOR ALL ZONE

BUCKLING = 0.0

REGION NUMBER AND ASSIGNMENT TO ZONE

REGION NO.	NAME	ZONE NO.	ZONE NAME	REGION NO.	NAME	ZONE NO.	ZONE NAME	REGION NO.	NAME	ZONE NO.	ZONE NAME	REGION NO.	NAME	ZONE NO.	ZONE NAME
1	IC	1	M1	2	OC	2	M2	3	RB	3	M3	4	CR	5	M5
5	CF	6	M6												

*** DIF3D (NODAL HEXAGONAL GEOMETRY OPTION) ***

*** NODAL PARAMETERS ***

4	IAPRX	ORDER OF NODAL APPROXIMATION IN HEX-PLANE
0	IAPRXZ	ORDER OF NODAL APPROXIMATION IN Z-DIRECTION
2	NCMI	NUMBER OF COARSE-MESH REBALANCE ITERATIONS PER OUTER ITERATION (-1 = NO COARSE-MESH REBALANCE)
0	ISEXTR	0/1 YES/NO ASYMPTOTIC SOURCE EXTRAPOLATION APPLIED TO OUTER ITERATIONS
0	NZSWP	NUMBER OF AXIAL PARTIAL CURRENT SWEEPS PER GROUP PER OUTER ITERATION

*** PROBLEM DESCRIPTION ***

NO. OF RINGS OF HEXAGONS	= 11
NO. OF 60 DEGREE SECTORS	= 1
NO. OF HEXAGONS IN PLANE	= 56
NO. OF ACTIVE HEXAGONS IN PLANE	= 49
NO. OF AXIAL PLANES	= 1
NO. OF HEXAGONAL-Z NODES	= 56
NO. OF UNIQUE NODE TYPES	= 5

*** DIF3D (NODAL OPTION) CYLINDER ALLOCATION ***

PROCEDURE PARAMETERS	DEFAULT CYLINDERS	RECOMMENDED CYLINDERS	DISK TYPE
ZONCYL	1	0	3330
FLXCYL	1	1	3330
PSICYL	5	1	3330
FDCCYL	20	1	3330
PSUCYL	3	1	3330
SRFCYL	12	1	3330
DMY1CYL	21	1	3330
DMY2CYL	7	3	3330
DMY5CYL	4	2	3330
RTCYL	5	1	3350
ATCYL	5	0	3350
NHCYL	5	1	3350
NACYL	5	0	3350

*** DIF3D (NODAL OPTION) STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	4000	5700
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH ALL DATA FOR 1 GROUP IN CORE	=	531	2393
WITH SCATTERING BAND OF FLUXES IN CORE	=	531	2551
WITH ALL FILES IN CORE (DURING OUTER ITERATIONS)	=	531	5014
WITH ALL FILES IN CORE (DURING EDIT OVERLAY)	=	531	5660

LOCATION OF SCRATCH FILES DURING OUTER ITERATIONS

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
FLUX MOMENTS	4	224	896	CORE	4
NEW HEX-PLANE PARTIAL CURRENTS	4	357	1428	CORE	4
OLD HEX-PLANE PARTIAL CURRENTS	4	357	1428	CORE	4
CROSS SECTIONS	4	72	288	CORE	4
NODAL COUPLING COEFFICIENTS	4	35	140	CORE	4

LOCATION OF SCRATCH FILES DURING EDIT OVERLAY

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NODE-AVERAGE FLUXES	4	100	400	CORE	4
FLUX SHAPE COEFFICIENTS	4	336	1344	CORE	4
FLUX MOMENTS	4	224	896	CORE	4
NEW HEX-PLANE PARTIAL CURRENTS	4	357	1428	CORE	4

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM	=	531	5660

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	KAPPA* PITCH	NO. OF INNERS	GROUP NO.	KAPPA* PITCH	NO. OF INNERS	GROUP NO.	KAPPA* PITCH	NO. OF INNERS	GROUP NO.	KAPPA* PITCH	NO. OF INNERS
1	1.211	2	2	0.732	4	3	1.862	2	4	1.906	2

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	FSRC. EXTRAP.	DOM. RATIO ESTIMATED	REBALANCE ERROR	K-EFFECTIVE
1	5.301356D+01	1.225204D+00	1.643987D-01	NO	2.037725D-01	5.819746D-01	1.16439865D+00
2	4.514973D+00	1.147041D-01	3.873655D-03	NO	1.865114D-01	5.533002D-02	1.16827231D+00
3	3.532498D-01	1.286835D-02	-1.515831D-02	NO	6.625057D-01	1.325572D-02	1.15311399D+00
4	1.117004D-01	5.333154D-03	-1.104645D-02	NO	7.899814D-01	2.053395D-02	1.14206754D+00
5	5.782048D-02	3.311817D-03	-7.160817D-03	NO	6.375314D-01	1.482393D-02	1.13490673D+00
6	3.326939D-02	1.920869D-03	-4.260461D-03	NO	5.744967D-01	8.790292D-03	1.13064626D+00
7	1.825124D-02	1.062688D-03	-2.401477D-03	NO	5.506851D-01	4.820466D-03	1.12824479D+00
8	9.890957D-03	5.794181D-04	-1.321340D-03	NO	5.450372D-01	2.577001D-03	1.12692345D+00
9	5.388163D-03	3.160789D-04	-7.243147D-04	YES	5.479299D-01	1.381935D-03	1.12619913D+00
10	1.538594D-03	1.092786D-04	-9.502524D-04	NO	3.391843D-01	1.013904D-04	1.12524888D+00
11	3.885185D-04	1.872911D-05	1.487498D-05	NO	1.338613D-01	2.404337D-05	1.12526376D+00
12	1.471937D-04	6.886788D-06	1.088369D-05	NO	4.516936D-01	1.280539D-05	1.12527464D+00
13	5.365769D-05	3.099757D-06	5.188913D-06	NO	5.105981D-01	8.303633D-06	1.12527983D+00
14	3.021890D-05	1.622623D-06	2.914471D-06	NO	5.398057D-01	5.356616D-06	1.12528274D+00
15	1.689288D-05	8.765365D-07	1.651698D-06	NO	5.474926D-01	3.281977D-06	1.12528439D+00
16	9.609086D-06	4.792744D-07	9.299330D-07	YES	5.478645D-01	1.925651D-06	1.12528532D+00
17	2.020246D-06	1.223496D-07	1.236097D-06	NO	2.563080D-01	2.373004D-07	1.12528656D+00
18	4.497027D-07	2.874515D-08	-1.727949D-08	NO	2.005760D-01	1.879097D-08	1.12528654D+00

OUTER ITERATIONS COMPLETED AT ITERATION 18, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.12528654279

MAXIMUM POWER DENSITY 2.69358D-04 OCCURS AT: RING NO. 1
POSITION NO. 1
SURFACE NO. 0
Z-COORDINATE = 0.0

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 2 **** 2D SNR BENCHMARK - RODS IN - NODAL 1/05/84 2222.600 PAGE 58

REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	IC	1	M1	1.43043D+03	1.00000D+00	2.87042D-01	2.00668D-04	2.69358D-04	1.34230D+00	5.74083D-01
2	OC	2	M2	1.52096D+03	1.00000D+00	2.03857D-01	1.34032D-04	2.26678D-04	1.69123D+00	4.07714D-01
3	RB	3	M3	1.95552D+03	1.00000D+00	9.10136D-03	4.65419D-06	1.82823D-05	3.92814D+00	1.82027D-02
4	CR	5	M5	2.17280D+02	1.00000D+00	0.0	0.0	0.0	0.0	0.0
5	CF	6	M6	1.08640D+02	1.00000D+00	0.0	0.0	0.0	0.0	0.0
	TOTALS			5.23283D+03	0.0	5.00000D-01	9.55506D-05	2.69358D-04	2.81901D+00	1.00000D+00

AREA NO.	AREA NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	TCORE	2.95139D+03	0.0	4.90899D-01	1.66328D-04	2.69358D-04	1.61944D+00	9.81797D-01
2	TROD	3.25920D+02	0.0	0.0	0.0	0.0	0.0	0.0
3	TOTAL	5.23283D+03	0.0	5.00000D-01	9.55506D-05	2.69358D-04	2.81901D+00	1.00000D+00

(1) INTEGRATION WEIGHT FACTOR = (?/B)*SIN(B*H) H=UNEXTRAPOLATED HALF HEIGHT, B=BUCKLING COEFFICIENT

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	IC	1	M1	1.00000D+00	1.00000D+00	1.00000D+00
2	OC	2	M2	6.00000D+00	1.00000D+00	1.00000D+00
3	RB	3	M3	8.00000D+00	1.00000D+00	1.00000D+00
4	CR	5	M5	0.0	0.0	0.0
5	CF	6	M6	0.0	0.0	0.0
	TOTALS			1.00000D+00	1.00000D+00	1.00000D+00

AREA NO.	AREA NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	TCORE	1.00000D+00	1.00000D+00	1.00000D+00
2	TROD	0.0	0.0	0.0
3	TOTAL	1.00000D+00	1.00000D+00	1.00000D+00

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 2 **** 2D SNR BENCHMARK - RODS IN - NODAL 1/05/84 2222.600 PAGE 59

MAXIMUM TOTAL FLUX 3.53887D+09 OCCURS AT: RING NO. 1
POSITION NO. 1
SURFACE NO. 0
Z-COORDINATE = 0.0

G.3 Sample Problem 3 (selected pages)

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 3 **** 3D SNR BENCHMARK - RODS IN - NODAL 1/05/84 2223.000 PAGE 84

*** DIF3D (NODAL OPTION) STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	20000	27000
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH ALL DATA FOR 1 GROUP IN CORE	=	594	26314
WITH SCATTERING BAND OF FLUXES IN CORE	=	594	26314
WITH ALL FILES IN CORE (DURING OUTER ITERATIONS)	=	594	47013
WITH ALL FILES IN CORE (DURING EDIT OVERLAY)	=	594	59338

LOCATION OF SCRATCH FILES DURING OUTER ITERATIONS

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
FLUX MOMENTS	4	2240	8960	CORE	4
NEW HEX-PLANE PARTIAL CURRENTS	4	2856	11424	DISK	1
NEW AXIAL PARTIAL CURRENTS	4	1008	4032	CORE	4
OLD HEX-PLANE PARTIAL CURRENTS	4	2856	11424	DISK	1
OLD AXIAL PARTIAL CURRENTS	4	1008	4032	DISK	1
CROSS SECTIONS	4	72	288	CORE	4
NODAL COUPLING COEFFICIENTS	4	117	468	CORE	4

LOCATION OF SCRATCH FILES DURING EDIT OVERLAY

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NODE-AVERAGE FLUXES	4	800	3200	DISK	1
FLUX SHAPE COEFFICIENTS	4	4032	16128	DISK	1
FLUX MOMENTS	4	2240	8960	DISK	1
NEW HEX-PLANE PARTIAL CURRENTS	4	2856	11424	DISK	1
NEW AXIAL PARTIAL CURRENTS	4	1008	4032	DISK	1

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM = 594 26853

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 3 **** 3D SNR BENCHMARK - RODS IN - NODAL 1/05/84 2223.000 PAGE 87

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	KAPPA* PITCH	NO. OF INNERS	GROUP NO.	KAPPA* PITCH	NO. OF INNERS	GROUP NO.	KAPPA* PITCH	NO. OF INNERS	GROUP NO.	KAPPA* PITCH	NO. OF INNERS
1	1.216	2	2	0.703	4	3	1.729	2	4	1.573	2

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	FSRC. EXTRAP.	DOM. RATIO ESTIMATED	REBALANCE ERROR	K-EFFECTIVE
1	4.115800D+02	1.882773D+00	-5.468500D-05	NO	3.024159D-01	5.313486D-01	9.99945315D-01
2	2.672773D+01	8.409265D-02	3.835296D-02	NO	2.702862D-01	7.047214D-02	1.03829828D+00
3	1.160805D+00	8.729627D-03	-1.142393D-02	NO	5.893127D-01	1.559124D-02	1.02687435D+00
4	2.298930D-01	2.070839D-03	-7.750840D-03	NO	5.811262D-01	1.170229D-02	1.01912351D+00
5	5.518316D-02	7.276864D-04	-4.019281D-03	NO	5.429634D-01	6.063665D-03	1.01510423D+00
6	2.789854D-02	4.976351D-04	-1.928680D-03	NO	5.502596D-01	3.922947D-03	1.01317555D+00
7	1.523165D-02	3.751465D-04	-8.745156D-04	YES	5.600124D-01	2.125458D-03	1.01230104D+00
8	1.051715D-02	1.452125D-04	-9.865616D-04	NO	2.874426D-01	5.627816D-04	1.01131447D+00
9	4.990391D-03	6.762131D-05	1.259094D-04	NO	4.852630D-01	2.319152D-04	1.01144038D+00
10	2.365442D-03	3.529278D-05	4.232512D-05	NO	6.223060D-01	1.470948D-04	1.01148271D+00
11	1.196305D-03	2.140311D-05	1.042653D-05	NO	6.289434D-01	9.649634D-05	1.01149314D+00
12	6.641565D-04	1.325022D-05	2.280020D-06	NO	5.867241D-01	5.895393D-05	1.01149542D+00
13	3.865679D-04	7.850677D-06	1.726237D-06	NO	5.493155D-01	3.282776D-05	1.01149714D+00
14	1.992933D-04	4.539753D-06	2.226419D-06	NO	5.317598D-01	1.917626D-05	1.01149937D+00
15	9.607115D-05	2.643282D-06	2.193967D-06	YES	5.357585D-01	1.087603D-05	1.01150156D+00
16	5.797460D-05	9.107678D-07	3.920518D-06	NO	4.196934D-01	2.329277D-06	1.01150548D+00
17	2.719733D-05	4.712384D-07	3.679485D-07	NO	4.702059D-01	1.301975D-06	1.01150585D+00
18	1.073510D-05	2.236516D-07	5.633647D-08	NO	5.043417D-01	8.163573D-07	1.01150591D+00
19	5.221894D-06	1.091903D-07	-5.154986D-08	NO	5.125455D-01	4.650900D-07	1.01150585D+00

OUTER ITERATIONS COMPLETED AT ITERATION 19, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.01150585498

MAXIMUM POWER DENSITY 3.03072D-06 OCCURS AT: RING NO. 1
POSITION NO. 1
SURFACE NO. 0
Z-COORDINATE = 8.51250D+01

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 3 **** 3D SNR BENCHMARK - RODS IN - NODAL 1/05/84 2223.600 PAGE 88

REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

REGION NO.	NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	AB	4	M4	2.36111D+05	1.00000D+00	6.84613D-03	2.89954D-08	1.75349D-07	6.04747D+00	1.36923D-02
2	IC	1	M1	1.35891D+05	1.00000D+00	2.63252D-01	1.93723D-06	3.03072D-06	1.56446D+00	5.26504D-01
3	OC	2	M2	1.44491D+05	1.00000D+00	2.18689D-01	1.51351D-06	2.89593D-06	1.91338D+00	4.37379D-01
4	RB	3	M3	3.42216D+05	1.00000D+00	1.12126D-02	3.27647D-08	2.68292D-07	8.18846D+00	2.24252D-02
5	CF	6	M6	3.36784D+04	1.00000D+00	0.0	0.0	0.0	0.0	0.0
6	CR	5	M5	2.33576D+04	1.00000D+00	0.0	0.0	0.0	0.0	0.0
	TOTALS			9.15745D+05	0.0	5.00000D-01	5.46003D-07	3.03072D-06	5.55074D+00	1.00000D+00

(1) INTEGRATION WEIGHT FACTOR = (2/B)*SIN(B*H) H=UNEXTRAPOLATED HALF HEIGHT, B=BUCKLING COEFFICIENT

REGION NO.	NAME	ZONE NO.	ZONE NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	AB	4	M4	1.00000D+00	1.00000D+00	2.00000D+00
2	IC	1	M1	1.00000D+00	1.00000D+00	4.00000D+00
3	OC	2	M2	6.00000D+00	1.00000D+00	4.00000D+00
4	RB	3	M3	8.00000D+00	1.00000D+00	4.00000D+00
5	CF	6	M6	0.0	0.0	0.0
6	CR	5	M5	0.0	0.0	0.0
	TOTALS			1.00000D+00	1.00000D+00	4.00000D+00

DIF3D 4.0 7/83 **** SAMPLE PROBLEM 3 **** 3D SNR BENCHMARK - RODS IN - NODAL 1/05/84 2223.600 PAGE 89

MAXIMUM TOTAL FLUX 3.95250D+07 OCCURS AT: RING NO. 1
POSITION NO. 1
SURFACE NO. 0
Z-COORDINATE = 8.51250D+01

G.4 Sample Problem 4 (selected pages)

DIF3D 4.0 1/84 **** SAMPLE PROBLEM 4 **** 3D SNR BENCHMARK - RODS IN - FD0636 1/23/84 1608.700 PAGE 104

*** DIF3D STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	12000	164000
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH 3 PLANES FOR 1 GROUP IN CORE	=	508	12225
WITH ALL DATA FOR 1 GROUP IN CORE	=	508	152345
WITH SCATTERING BAND OF FLUXES IN CORE	=	508	205913
WITH ALL FILES IN CORE	=	508	438257

LOCATION OF SCRATCH FILES DURING STEADY STATE CALCULATION

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NEW FISSION SOURCE	1	17856	17856	CORE	1
OLD FISSION SRC. 1	1	17856	17856	CORE	1
OLD FISSION SRC. 2	1	17856	17856	DISK	0
TOTAL SOURCE	1	17856	17856	CORE	1
COMPOSITION MAP	1	8928	8928	CORE	1
FLUX ITERATE	4	17856	71424	DISK	1
CROSS SECTIONS	4	72	288	CORE	4
FINITEDIFF. COEFS.	4	71424	285696	DISK	1

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM = 508 152561

DIF3D 4.0 1/84 **** SAMPLE PROBLEM 4 **** 3D SNR BENCHMARK - RODS IN - FD0636 1/23/84 1608.900 PAGE 108

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS
1	1.52724D+00	10	2	1.66503D+00	14	3	1.39934D+00	7	4	1.47889D+00	8

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
1	5.908024D-01	2.179524D-01	-3.875600D-02	0	0.0	0.0	9.61244003D-01
2	6.733313D-01	2.024667D-01	2.106814D-02	0	0.0	9.913276D-01	9.82312139D-01
3	4.764514D-01	7.901021D-02	1.674584D-02	0	0.0	4.377587D-01	9.99057983D-01
4	1.888638D-01	4.227813D-02	7.057055D-03	1	4.377587D-01	4.377587D-01	1.00611504D+00
5	5.631559D-02	2.039071D-02	3.679833D-03	2	4.377587D-01	6.037430D-01	1.00979487D+00
6	2.921216D-02	9.729249D-03	1.783028D-03	3	4.377587D-01	6.227869D-01	1.01157790D+00
7	1.735153D-02	4.993231D-03	7.183110D-04	1	6.227869D-01	6.227869D-01	1.01229621D+00
8	7.881610D-03	2.386063D-03	3.047675D-04	2	6.227869D-01	6.411442D-01	1.01260098D+00
9	2.209185D-03	7.190380D-04	1.613694D-04	3	6.227869D-01	6.430465D-01	1.01276235D+00
10	2.072177D-03	2.778078D-04	3.904903D-05	1	6.430465D-01	6.430465D-01	1.01280140D+00
11	5.335848D-04	1.518552D-04	4.664759D-06	2	6.430465D-01	6.924204D-01	1.01280606D+00
12	1.513701D-04	5.494587D-05	2.434434D-06	3	6.430465D-01	6.855575D-01	1.01280850D+00
13	2.044381D-04	2.275005D-05	-2.503817D-06	1	6.855575D-01	6.855575D-01	1.01280599D+00
14	3.648853D-05	1.282983D-05	-1.270115D-06	2	6.855575D-01	7.134172D-01	1.01280472D+00
15	1.588739D-05	4.165014D-06	-3.767691D-07	3	6.855575D-01	6.992496D-01	1.01280434D+00
16	1.772728D-05	1.480040D-06	-5.193528D-07	1	6.992496D-01	6.992496D-01	1.01280383D+00
17	3.512971D-06	8.225556D-07	-1.774384D-07	2	6.992496D-01	7.110809D-01	1.01280365D+00
18	1.530163D-06	2.493004D-07	-4.614461D-08	3	6.992496D-01	6.990136D-01	1.01280360D+00

OUTER ITERATIONS COMPLETED AT ITERATION 18, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.01280360172

DIF3D 4.0 1/84 **** SAMPLE PROBLEM 4 **** 3D SNR BENCHMARK - RODS IN - FD0636 1/23/84 1610.200 PAGE 109

TO RESTART THIS CALCULATION, INPUT FOLLOWING VALUES

DOMINANCE RATIO (SIGBAR) = 6.990136498443D-01

OPTIMIZED OVER-RELAXATION FACTORS

GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA
1	1.52724D+00	2	1.66503D+00	3	1.39934D+00	4	1.47889D+00		

ERROR COUNT

SUBROUTINE	ERROR NO.	TYPE	NO. OF ERRORS
ORPES1	100	NONFATAL	2

MAXIMUM POWER DENSITY 3.01935D-06 OCCURS AT MESH CELL (I,J,K) = (1, 1, 18)

PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX VALUES ON THE CELL SURFACES AND WITHIN THE CELL.

DIF3D 4.0 1/84 **** SAMPLE PROBLEM 4 **** 3D SNR BENCHMARK - RODS IN - FD0636 1/23/84 1613.800 PAGE 110

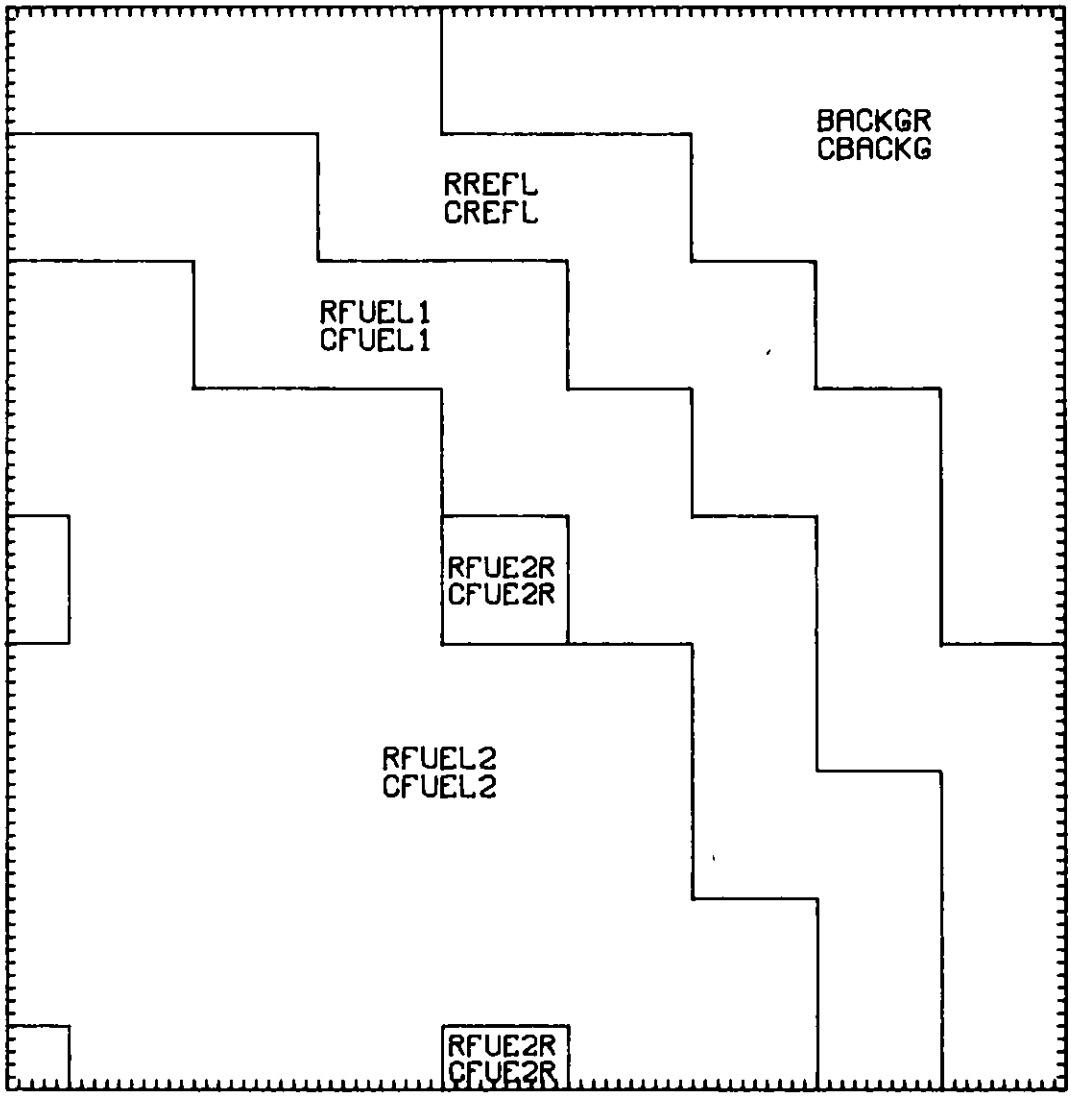
REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.050D+07)

REGION NO.	NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	AB	4	M4	2.36111D+05	1.00000D+00	6.79240D-03	2.87678D-08	1.76254D-07	6.12676D+00	1.35848D-02
2	IC	1	M1	1.35891D+05	1.00000D+00	2.62993D-01	1.93533D-06	3.01935D-06	1.56012D+00	5.25986D-01
3	OC	2	M2	1.44491D+05	1.00000D+00	2.19122D-01	1.51651D-06	2.89991D-06	1.91223D+00	4.38244D-01
4	RB	3	M3	3.42216D+05	1.00000D+00	1.10924D-02	3.24135D-08	2.64958D-07	8.17431D+00	2.21849D-02
5	CF	6	M6	3.36784D+04	1.00000D+00	0.0	0.0	0.0	0.0	0.0
6	CR	5	M5	2.33576D+04	1.00000D+00	0.0	0.0	0.0	0.0	0.0
	TOTALS			9.15745D+05	0.0	5.00000D-01	5.46004D-07	3.01935D-06	5.52991D+00	1.00000D+00

(1) INTEGRATION WEIGHT FACTOR = (2/B)*SIN(B*H) H=UNEXTRAPOLATED HALF HEIGHT, B=BUCKLING COEFFICIENT
(2) THE PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX ON THE CELL SURFACES AND WITHIN THE CELL.

REGION NO.	NAME	ZONE NO.	ZONE NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	AB	4	M4	1.00000D+00	1.00000D+00	8.00000D+00
2	IC	1	M1	1.00000D+00	1.00000D+00	1.80000D+01
3	OC	2	M2	1.00000D+01	5.00000D+00	1.70000D+01
4	RB	3	M3	1.40000D+01	7.00000D+00	1.70000D+01
5	CF	6	M6	0.0	0.0	0.0
6	CR	5	M5	0.0	0.0	0.0
	TOTALS			1.00000D+00	1.00000D+00	1.80000D+01

G.5 Sample Problem (selected pages)



GNIP4C Generated Calcomp 780 Plot of 2D IAEA Benchmark Model

DIF3D 4.0 7/83 **** SAMPLE 5 **** IAEA 2D BENCHMARK - 2. CM MESH 1/05/84 1616.300 PAGE 14

*** DIF3D STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	200	102000
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH ALL DATA FOR 1 GROUP IN CORE	=	790	61464
WITH SCATTERING BAND OF FLUXES IN CORE	=	790	68689
WITH ALL FILES IN CORE	=	790	97639

LOCATION OF SCRATCH FILES DURING STEADY STATE CALCULATION

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NEW FISSION SOURCE	1	7225	7225	CORE	1
OLD FISSION SRC. 1	1	7225	7225	CORE	1
OLD FISSION SRC. 2	1	7225	7225	CORE	1
TOTAL SOURCE	1	7225	7225	CORE	1
COMPOSITION MAP	1	3613	3613	CORE	1
FLUX ITERATE	2	7225	14450	CORE	2
CROSS SECTIONS	2	50	100	CORE	2
FINITEDIFF. COEFS.	2	21675	43350	CORE	2

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM = 790 97639

DIF3D 4.0 7/83 **** SAMPLE 5 **** IAEA 2D BENCHMARK - 2. CM MESH 1/05/84 1616.400 PAGE 25

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS
1	1.56620D+00	14	2	1.41751D+00	9						

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
1	3.686295D-01	8.812177D-02	1.224134D-02	0	0.0	0.0	1.01224134D+00
2	1.087090D-01	4.075031D-02	1.235995D-02	0	0.0	4.695831D-01	1.02460129D+00
3	5.541415D-02	2.380535D-02	1.054773D-03	0	0.0	5.912010D-01	1.02565606D+00
4	3.550666D-02	1.769028D-02	6.707207D-04	1	5.912010D-01	5.912010D-01	1.02632678D+00
5	2.726305D-02	1.274709D-02	6.574164D-04	2	5.912010D-01	8.050748D-01	1.02698420D+00
6	2.324552D-02	9.655415D-03	5.224960D-04	3	5.912010D-01	8.363244D-01	1.02750669D+00
7	1.954620D-02	8.190440D-03	3.320014D-04	1	8.363244D-01	8.363244D-01	1.02783870D+00
8	1.603185D-02	7.109886D-03	2.622962D-04	2	8.363244D-01	9.241546D-01	1.02810099D+00
9	1.118446D-02	5.623376D-03	3.391927D-04	3	8.363244D-01	9.287023D-01	1.02844018D+00
10	9.360004D-03	4.863033D-03	2.143255D-04	1	9.287023D-01	9.287023D-01	1.02865451D+00
11	8.528902D-03	4.580230D-03	1.056055D-04	2	9.287023D-01	9.694433D-01	1.02876012D+00
12	6.183622D-03	3.634297D-03	2.077926D-04	3	9.287023D-01	9.564793D-01	1.02896791D+00
13	5.174504D-03	2.940846D-03	1.482553D-04	1	9.564793D-01	9.564793D-01	1.02911616D+00
14	4.992018D-03	2.944204D-03	3.461179D-05	2	9.564793D-01	1.001017D+00	1.02915078D+00
15	3.613034D-03	2.318619D-03	9.803535D-05	3	9.564793D-01	9.673322D-01	1.02924881D+00
16	3.187787D-03	1.740132D-03	7.516984D-05	1	9.673322D-01	9.673322D-01	1.02932398D+00
17	3.137347D-03	1.811439D-03	1.251830D-05	2	9.673322D-01	1.021432D+00	1.02933650D+00
18	2.267487D-03	1.398910D-03	4.055590D-05	3	9.673322D-01	9.710263D-01	1.02937705D+00
19	2.010706D-03	9.980777D-04	3.302212D-05	1	9.710263D-01	9.710263D-01	1.02941008D+00
20	1.855544D-03	1.060073D-03	7.416327D-06	2	9.710263D-01	1.032139D+00	1.02941749D+00
21	1.342631D-03	8.123937D-04	1.612011D-05	3	9.710263D-01	9.729018D-01	1.02943361D+00
22	1.279728D-03	5.653021D-04	1.323734D-05	1	9.729018D-01	9.729018D-01	1.02944685D+00
23	1.090173D-03	6.093860D-04	4.703061D-06	2	9.729018D-01	1.040157D+00	1.02945156D+00

DIF3D 4.0 7/83 **** SAMPLE 5 **** IAEA 2D BENCHMARK - 2. CM MESH 1/05/84 1617.200 PAGE 26

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
24	7.869962D-04	4.639558D-04	6.597291D-06	3	9.729018D-01	9.740612D-01	1.02945815D+00
25	7.970648D-04	3.202154D-04	5.286035D-06	1	9.740612D-01	9.740612D-01	1.02946344D+00
26	6.211472D-04	3.447927D-04	2.756975D-06	2	9.740612D-01	1.039436D+00	1.02946620D+00
27	4.495778D-04	2.624991D-04	2.867366D-06	3	9.740612D-01	9.740058D-01	1.02946906D+00
28	4.981576D-04	1.793089D-04	2.168207D-06	4	9.740612D-01	9.656760D-01	1.02947123D+00
29	2.378958D-04	1.218137D-04	3.231051D-06	5	9.740612D-01	9.661532D-01	1.02947446D+00
30	1.547608D-04	6.771766D-05	1.876176D-06	6	9.740612D-01	9.647719D-01	1.02947634D+00
31	1.121440D-04	4.944923D-05	1.483748D-06	7	9.740612D-01	9.675397D-01	1.02947782D+00
32	5.678522D-05	2.690326D-05	1.101921D-06	8	9.740612D-01	9.675678D-01	1.02947892D+00
33	3.057508D-05	2.255934D-05	4.901346D-07	9	9.740612D-01	9.696887D-01	1.02947941D+00
34	1.619595D-05	1.594660D-05	2.568945D-07	10	9.740612D-01	9.705203D-01	1.02947967D+00
35	1.375732D-05	1.287818D-05	1.301539D-07	11	9.740612D-01	9.715116D-01	1.02947980D+00
36	1.186071D-05	1.120915D-05	1.520512D-08	12	9.740612D-01	9.724532D-01	1.02947982D+00
37	9.942655D-06	8.340138D-06	-3.135238D-08	13	9.740612D-01	9.727809D-01	1.02947979D+00

OUTER ITERATIONS COMPLETED AT ITERATION 37, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.02947978522

TO RESTART THIS CALCULATION, INPUT FOLLOWING VALUES

DOMINANCE RATIO (SIGBAR) = 9.727808648906D-01

OPTIMIZED OVER-RELAXATION FACTORS

GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA
NO.	OMEGA								
1	1.56620D+00	2	1.41751D+00						

DIF3D 4.0 7/83 **** SAMPLE 5 **** IAEA 2D BENCHMARK - 2. CM MESH 1/05/84 1617.200 PAGE 27

MAXIMUM POWER DENSITY 8.67119D-05 OCCURS AT MESH CELL (I,J,K) = (16, 16, 1)

PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX VALUES ON THE CELL SURFACES AND WITHIN THE CELL.

DIF3D 4.0 7/83 **** SAMPLE 5 **** IAEA 2D BENCHMARK - 2. CM MESH 1/05/84 1627.100 PAGE 28

REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.000D+07)

REGION NO.	NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	RREFL	4	CREFL	6.40000D+03	1.00000D+00	0.0	0.0	0.0	0.0	0.0
2	RFUEL1	1	CFUEL1	5.60000D+03	1.00000D+00	2.29781D-01	4.10324D-05	8.60665D-05	2.09753D+00	2.29781D-01
3	RFUEL2	2	CFUEL2	1.12000D+04	1.00000D+00	7.41689D-01	6.62222D-05	8.67119D-05	1.30941D+00	7.41689D-01
4	RFUE2R	3	CFUE2R	9.00000D+02	1.00000D+00	2.85301D-02	3.17001D-05	5.89426D-05	1.85939D+00	2.85301D-02
5	BACKGR	5	CBACKG	4.80000D+03	1.00000D+00	0.0	0.0	0.0	0.0	0.0
	TOTALS			2.89000D+04	0.0	1.00000D+00	3.46021D-05	8.67119D-05	2.50597D+00	1.00000D+00

AREA NO.	AREA NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	TFUEL	1.68000D+04	0.0	9.71470D-01	5.78256D-05	8.67119D-05	1.49954D+00	9.71470D-01

(1) INTEGRATION WEIGHT FACTOR = (2/B)*SIN(B*H) H=UNEXTRAPOLATED HALF HEIGHT, B=BUCKLING COEFFICIENT
(2) THE PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX ON THE CELL SURFACES AND WITHIN THE CELL.

REGION NO.	NAME	ZONE NO.	ZONE NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	RREFL	4	CREFL	0.0	0.0	0.0
2	RFUEL1	1	CFUEL1	2.80000D+01	6.50000D+01	1.00000D+00
3	RFUEL2	2	CFUEL2	1.60000D+01	1.60000D+01	1.00000D+00
4	RFUE2R	3	CFUE2R	5.00000D+00	5.00000D+00	1.00000D+00
5	BACKGR	5	CBACKG	0.0	0.0	0.0
	TOTALS			1.60000D+01	1.60000D+01	1.00000D+00

AREA NO.	AREA NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	TFUEL	1.60000D+01	1.60000D+01	1.00000D+00

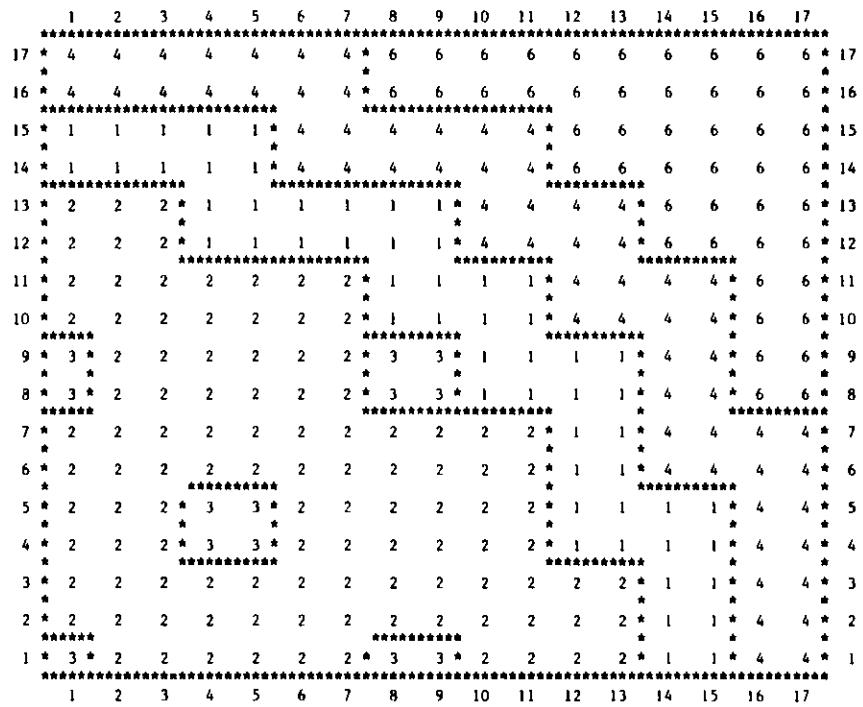
G.6 Sample Problem 6 (selected pages)

GN1P4C 11/83 **** BENCHMARK PROBLEM 6 **** IAEA 3D BENCHMARK 10. CM MESH 1/05/84 1628.000 PAGE 44

REACTOR COMPOSITION MAP

Z-DIM MAP FOR PLANES 29 - 36

Y -DIM /X -DIM



DIF3D 4.0 7/83 **** BENCHMARK PROBLEM 6 **** IAEA 3D BENCHMARK 10. CM MESH 1/17/84 1044.700 PAGE 51

*** DIF3D STORAGE ALLOCATION ***

		FCM	ECM
NUMBER OF WORDS IN DATA STORAGE CONTAINER	=	8000	166000
MINIMUM NUMBER OF WORDS REQUIRED TO RUN THIS PROBLEM			
WITH 3 PLANES FOR 1 GROUP IN CORE	=	390	7142
WITH ALL DATA FOR 1 GROUP IN CORE	=	390	93697
WITH SCATTERING BAND OF FLUXES IN CORE	=	390	104679
WITH ALL FILES IN CORE	=	390	159649

LOCATION OF SCRATCH FILES DURING STEADY STATE CALCULATION

FILE CONTENTS	NO. OF RECORDS	RECORD LENGTH	FILE LENGTH	LOCATION	RECORDS IN CORE
NEW FISSION SOURCE	1	10982	10982	CORE	1
OLD FISSION SRC. 1	1	10982	10982	CORE	1
OLD FISSION SRC. 2	1	10982	10982	CORE	1
TOTAL SOURCE	1	10982	10982	CORE	1
COMPOSITION MAP	1	5491	5491	CORE	1
FLUX ITERATE	2	10982	21964	CORE	1
CROSS SECTIONS	2	60	120	CORE	1
FINITEDIFF. COEFS.	2	43928	87856	CORE	1

TOTAL NUMBER OF WORDS USED FOR THIS PROBLEM	=	390	159649

DIF3D 4.0 7/83 **** BENCHMARK PROBLEM 6 **** IAEA 3D BENCHMARK 10. CM MESH 1/17/84 1044.800 PAGE 63

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OPTIMIZED INNER ITERATION STRATEGY

GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS	GROUP NO.	OPTIMUM OMEGA	NO. OF INNERS
1	1.16565D+00	5	2	1.08039D+00	4						

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
1	2.771832D-01	1.024438D-01	3.830969D-03	0	0.0	0.0	1.00383097D+00
2	1.760958D-01	5.806885D-02	1.040214D-02	0	0.0	5.729916D-01	1.01423311D+00
3	1.198757D-01	3.941884D-02	3.010733D-03	0	0.0	6.892115D-01	1.01724384D+00
4	9.499101D-02	3.088157D-02	1.957533D-03	1	6.892115D-01	6.892115D-01	1.01920138D+00
5	6.828438D-02	2.328266D-02	2.019535D-03	2	6.892115D-01	8.443129D-01	1.02122093D+00
6	4.924479D-02	1.784312D-02	1.744825D-03	3	6.892115D-01	8.720990D-01	1.02296576D+00
7	4.094458D-02	1.525653D-02	1.071401D-03	1	8.720990D-01	8.720990D-01	1.02403716D+00
8	3.579333D-02	1.357514D-02	7.486434D-04	2	8.720990D-01	9.410850D-01	1.02478580D+00
9	2.692639D-02	1.098765D-02	1.034374D-03	3	8.720990D-01	9.445983D-01	1.02582017D+00
10	2.109728D-02	9.372968D-03	7.241987D-04	1	9.445983D-01	9.445983D-01	1.02654437D+00
11	2.019927D-02	8.789725D-03	3.378608D-04	2	9.445983D-01	9.695127D-01	1.02688223D+00
12	1.739404D-02	7.245002D-03	5.705062D-04	3	9.445983D-01	9.649009D-01	1.02745274D+00
13	1.417056D-02	5.861442D-03	4.926338D-04	1	9.649009D-01	9.649009D-01	1.02794537D+00
14	1.337218D-02	5.642111D-03	1.675143D-04	2	9.649009D-01	9.823799D-01	1.02811289D+00
15	1.095615D-02	4.658183D-03	2.441338D-04	3	9.649009D-01	9.705796D-01	1.02835702D+00
16	8.621393D-03	3.596802D-03	2.380209D-04	1	9.705796D-01	9.705796D-01	1.02859504D+00
17	8.442859D-03	3.506622D-03	6.598459D-05	2	9.705796D-01	9.883116D-01	1.02868103D+00
18	7.214700D-03	2.876718D-03	8.820695D-05	3	9.705796D-01	9.715993D-01	1.02876923D+00
19	5.804683D-03	2.170280D-03	9.339572D-05	1	9.715993D-01	9.715993D-01	1.02886263D+00
20	5.543135D-03	2.124218D-03	4.543612D-05	2	9.715993D-01	9.898949D-01	1.02890807D+00
21	4.485072D-03	1.737412D-03	2.830801D-05	3	9.715993D-01	9.714718D-01	1.02893637D+00
22	3.474716D-03	1.305627D-03	3.380435D-05	4	9.715993D-01	9.690728D-01	1.02897018D+00
23	2.604693D-03	9.424705D-04	2.811508D-05	5	9.715993D-01	9.690368D-01	1.02899829D+00

DIF3D 4.0 7/83 **** BENCHMARK PROBLEM 6 **** IAEA 3D BENCHMARK 10. CM MESH 1/17/84 1044.900 PAGE 64

OUTER ITERATION SUMMARY REAL SOLUTION K-EFF. PROBLEM

OUTER IT. NO.	REL. POINT ERROR	REL. SUM ERROR	EIGENVALUE CHANGE	POLY. ORDER	DOM. RATIO USED	DOM. RATIO ESTIMATED	K-EFFECTIVE
24	1.937053D-03	6.607192D-04	1.991767D-05	6	9.715993D-01	9.692004D-01	1.02901821D+00
25	1.411882D-03	4.769696D-04	1.310000D-05	7	9.715993D-01	9.699473D-01	1.02903131D+00
26	9.602456D-04	3.509318D-04	8.562595D-06	8	9.715993D-01	9.706147D-01	1.02903987D+00
27	6.607808D-04	2.807478D-04	5.600065D-06	9	9.715993D-01	9.717033D-01	1.02904547D+00
28	5.090272D-04	2.340001D-04	3.640009D-06	1	9.717033D-01	9.717033D-01	1.02904911D+00
29	5.108685D-04	2.410647D-04	2.855307D-06	2	9.717033D-01	1.015566D+00	1.02905197D+00
30	4.819845D-04	2.155923D-04	8.128949D-07	3	9.717033D-01	9.887233D-01	1.02905278D+00
31	4.476779D-04	1.898788D-04	7.823396D-07	1	9.887233D-01	9.887233D-01	1.02905356D+00
32	4.472955D-04	1.905386D-04	-1.469485D-07	2	9.887233D-01	1.001790D+00	1.02905342D+00
33	3.860226D-04	1.707806D-04	7.510760D-07	3	9.887233D-01	9.865745D-01	1.02905417D+00
34	3.365650D-04	1.444165D-04	8.173546D-07	4	9.887233D-01	9.843849D-01	1.02905499D+00
35	2.905289D-04	1.190343D-04	7.129103D-07	5	9.887233D-01	9.846099D-01	1.02905570D+00
36	2.333374D-04	9.505854D-05	5.250085D-07	6	9.887233D-01	9.849260D-01	1.02905622D+00
37	1.865328D-04	7.591994D-05	3.521412D-07	7	9.887233D-01	9.855128D-01	1.02905658D+00
38	1.402165D-04	6.036084D-05	2.159031D-07	8	9.887233D-01	9.860203D-01	1.02905679D+00
39	1.010335D-04	4.793465D-05	1.020897D-07	9	9.887233D-01	9.864420D-01	1.02905689D+00
40	8.130474D-05	3.839384D-05	2.132365D-08	10	9.887233D-01	9.868250D-01	1.02905692D+00
41	6.432867D-05	2.976832D-05	-3.466991D-08	11	9.887233D-01	9.870009D-01	1.02905688D+00
42	4.754541D-05	2.341330D-05	-7.725147D-08	12	9.887233D-01	9.872028D-01	1.02905680D+00
43	3.553214D-05	1.726704D-05	-1.005624D-07	13	9.887233D-01	9.872144D-01	1.02905670D+00
44	2.655172D-05	1.300379D-05	-1.092027D-07	14	9.887233D-01	9.872958D-01	1.02905659D+00
45	1.836076D-05	9.043078D-06	-1.104239D-07	15	9.887233D-01	9.872579D-01	1.02905648D+00
46	1.368597D-05	6.435247D-06	-1.032808D-07	16	9.887233D-01	9.872922D-01	1.02905638D+00
47	1.028656D-05	4.436357D-06	-9.063790D-08	17	9.887233D-01	9.873148D-01	1.02905629D+00
48	8.778839D-06	3.019638D-06	-7.653597D-08	18	9.887233D-01	9.873501D-01	1.02905621D+00

DIF3D 4.0 7/83 **** BENCHMARK PROBLEM 6 **** IAEA 3D BENCHMARK 10. CM MESH 1/17/84 1044.900 PAGE 65

OUTER ITERATIONS COMPLETED AT ITERATION 48, ITERATIONS HAVE CONVERGED

K-EFFECTIVE = 1.02905621257

TO RESTART THIS CALCULATION, INPUT FOLLOWING VALUES

DOMINANCE RATIO (SIGBAR) = 9.873501094068D-01

OPTIMIZED OVER-RELAXATION FACTORS

GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA	GROUP NO.	OPTIMUM OMEGA
1	1.16565D+00	2	1.08039D+00						

MAXIMUM POWER DENSITY 4.29119D-07 OCCURS AT MESH CELL (I,J,K) = (4, 3, 18)

PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX VALUES ON THE CELL SURFACES AND WITHIN THE CELL.

DIF3D 4.0 7/83 **** BENCHMARK PROBLEM 6 **** IAEA 3D BENCHMARK 10. CM MESH 1/17/84 1046.300 PAGE 66

REGION AND AREA POWER INTEGRALS FOR K-EFF PROBLEM WITH ENERGY RANGE (EV) =(0.0 ,1.000D+07)

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	RREFL	4	CREFL	3.11400D+06	1.00000D+00	0.0	0.0	0.0	0.0	0.0
2	RFUEL1	1	CFUEL1	1.90400D+06	1.00000D+00	2.06648D-01	1.08534D-07	3.45221D-07	3.18078D+00	2.06648D-01
3	RFUEL2	2	CFUEL2	3.77600D+06	1.00000D+00	7.64862D-01	2.02559D-07	4.29119D-07	2.11849D+00	7.64862D-01
4	RFUE2R	3	CFUE2R	3.38000D+05	1.00000D+00	2.84906D-02	8.42918D-08	2.77697D-07	3.29447D+00	2.84906D-02
5	RREFLR	5	CREFLR	2.60000D+04	1.00000D+00	0.0	0.0	0.0	0.0	0.0
6	BACKGR	6	CBACKG	1.82400D+06	1.00000D+00	0.0	0.0	0.0	0.0	0.0
	TOTALS			1.09820D+07	0.0	1.00000D+00	9.10581D-08	4.29119D-07	4.71258D+00	1.00000D+00

AREA NO.	AREA NAME	VOLUME (CC)	INTEGRATION(1) WEIGHT FACTOR	POWER (WATTS)	POWER DENSITY (WATTS/CC)	PEAK DENSITY (WATTS/CC)(2)	PEAK TO AVG. POWER DENSITY	POWER FRACTION
1	TFUEL	5.68000D+06	0.0	9.71509D-01	1.71040D-07	4.29119D-07	2.50887D+00	9.71509D-01

(1) INTEGRATION WEIGHT FACTOR = (2/B)*SIN(B*H) H=UNEXTRAPOLATED HALF HEIGHT, B=BUCKLING COEFFICIENT
(2) THE PEAK POWER DENSITY IS CALCULATED BY SAMPLING THE AVERAGE FLUX ON THE CELL SURFACES AND WITHIN THE CELL.

REGION NO.	REGION NAME	ZONE NO.	ZONE NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'
1	RREFL	4	CREFL	0.0	0.0	0.0
2	RFUEL1	1	CFUEL1	1.30000D+01	6.00000D+00	1.80000D+01
3	RFUEL2	2	CFUEL2	4.00000D+00	3.00000D+00	1.80000D+01
4	RFUE2R	3	CFUE2R	1.00000D+00	1.00000D+00	1.80000D+01
5	RREFLR	5	CREFLR	0.0	0.0	0.0
6	BACKGR	6	CBACKG	0.0	0.0	0.0
	TOTALS			4.00000D+00	3.00000D+00	1.80000D+01

AREA NO.	AREA NAME	PEAK INDEX 'X'	PEAK INDEX 'Y'	PEAK INDEX 'Z'	POWER DENSITY AXIAL (3)	PEAK TO AVG. P.D. AXIAL (3)
1	TFUEL	4.00000D+00	3.00000D+00	1.80000D+01	2.64605D-07	1.62174D+00

(3) DERIVED FROM DATA IN THE AXIAL COLUMN OF MESH CELLS THAT INTERSECTS THE REACTOR PEAK POWER DENSITY LOCATION

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